

Transport and a Goldilocks Search

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Climate, Ocean, and Sea Ice Modeling Project
<http://public.lanl.gov/ringler/ringler.html>

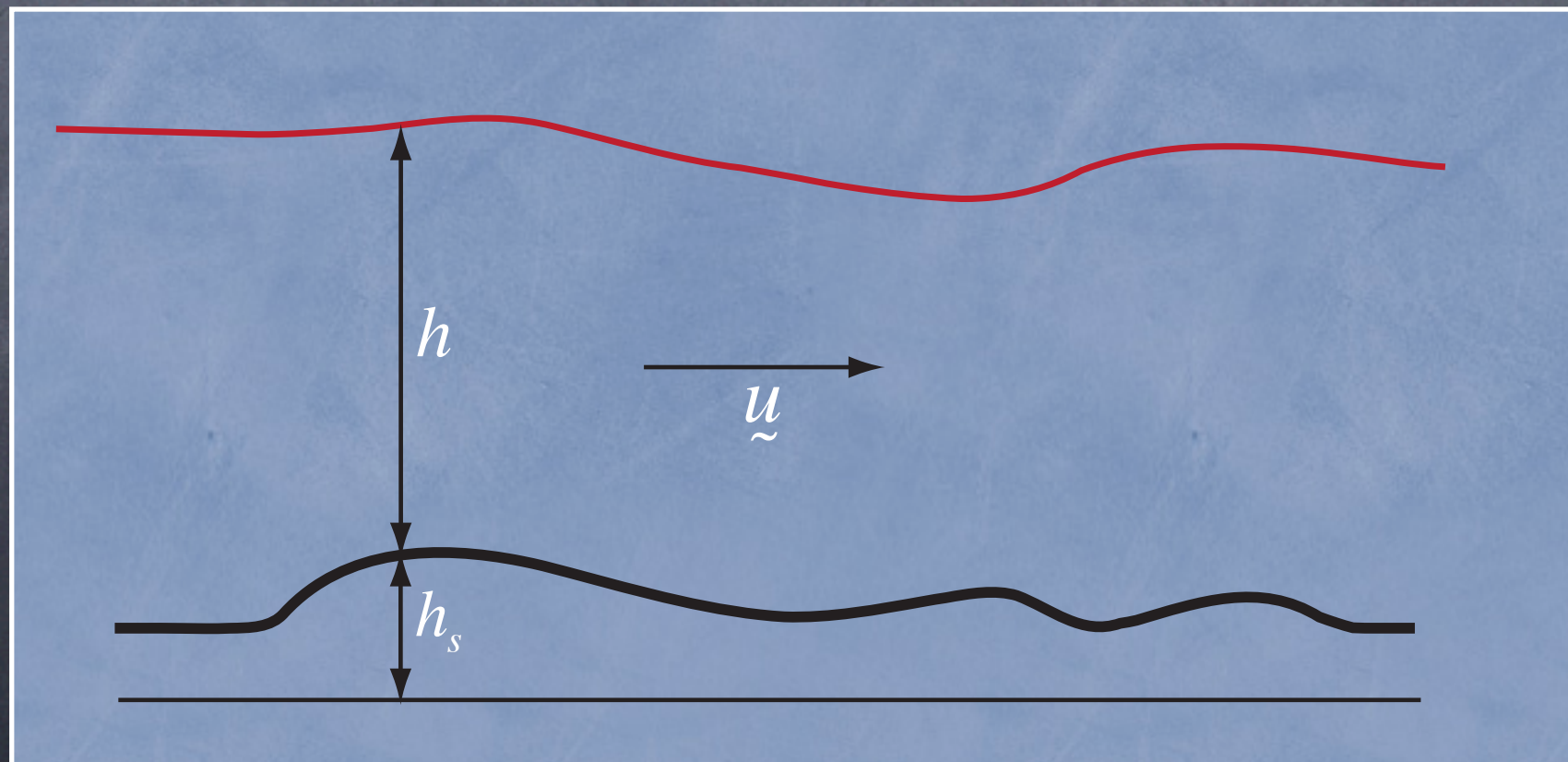
First, let's define our equations.

$$\frac{\partial h}{\partial t} + \nabla \cdot (h \underline{u}) = 0 \quad \text{thickness plays the role of pressure (uniform density).}$$

$$\frac{\partial \underline{u}}{\partial t} + (\omega + f) \underline{k} \times \underline{u} = -g \nabla (h + h_s) - \frac{1}{2} \nabla \|\underline{u}\|^2 \quad \text{velocity is in the tangent plane.}$$

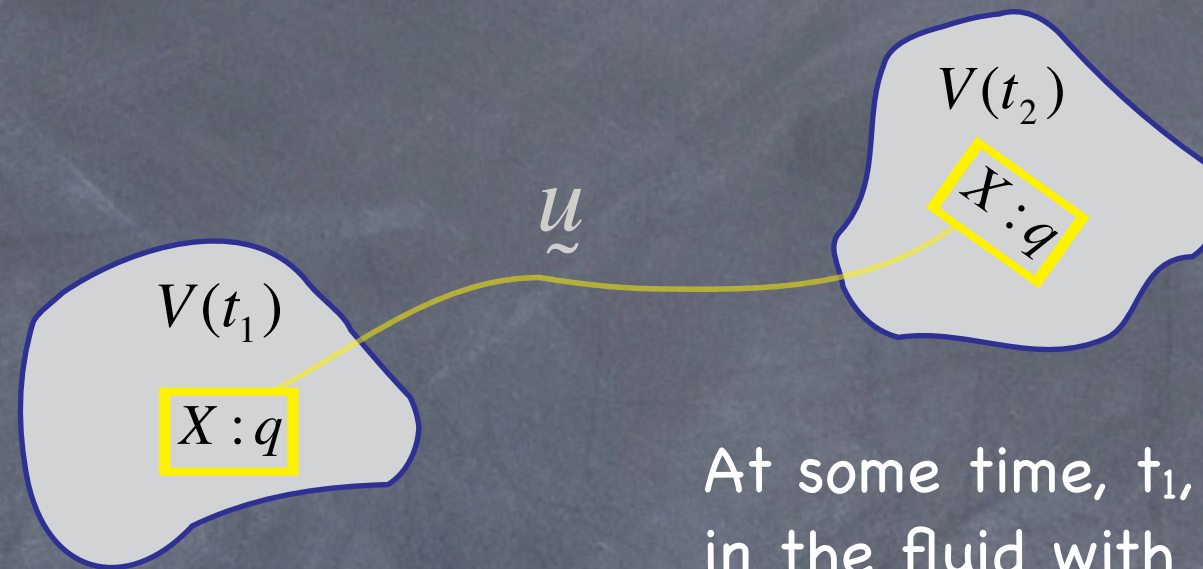
$$\omega = \underline{k} \cdot (\nabla \times \underline{u}) \quad \text{only keep track of the vertical component of vorticity.}$$

$$\eta = \omega + f \quad \text{definition of absolute vorticity.}$$



And add tracer transport

$$\frac{Dq}{Dt} = 0$$



At some time, t_1 , we tag all particles in the fluid with an additional label that represents the value of the tracer (q) field.

This label is “conserved” (i.e. does not change) as the particle moves through the fluid, thus (by definition): $Dq/Dt = 0$.

Note that q is a concentration, i.e. q has units of $\text{kg}_{\text{something}}/\text{kg}_{\text{mass}}$.

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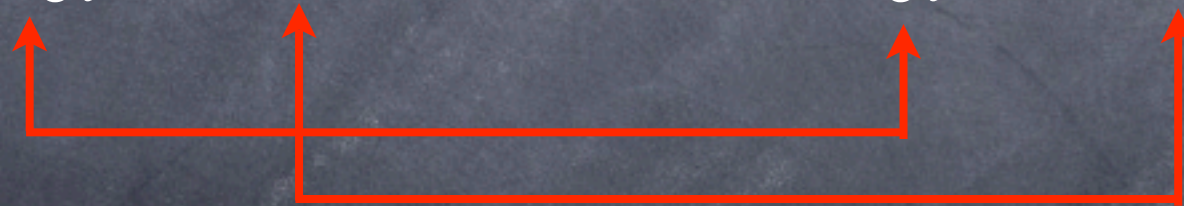
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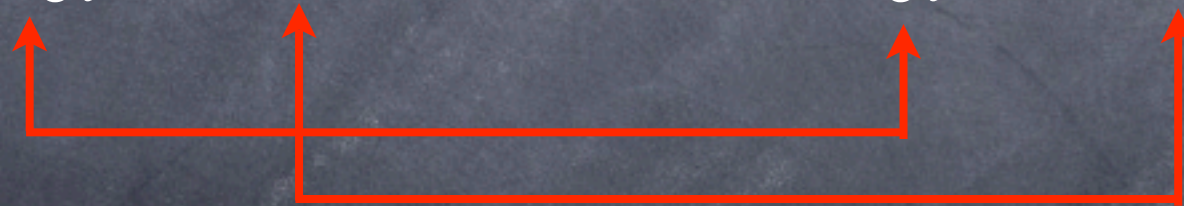
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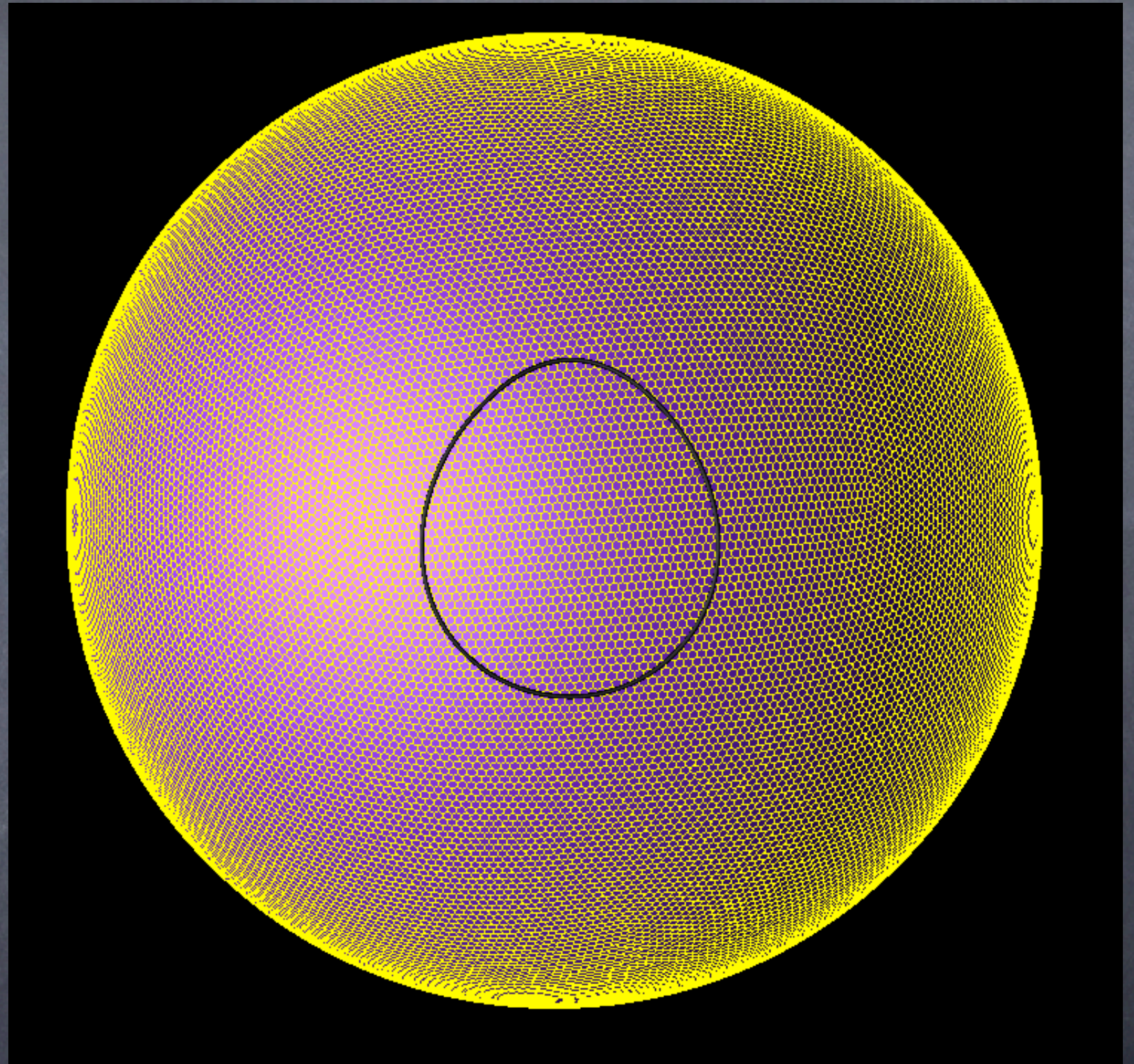
Next, let's define our physical setting.

The SW equations are discretized on the sphere.

There is a mountain located at 30N. As we will see, this mountain protrudes through the fluid to create an island.

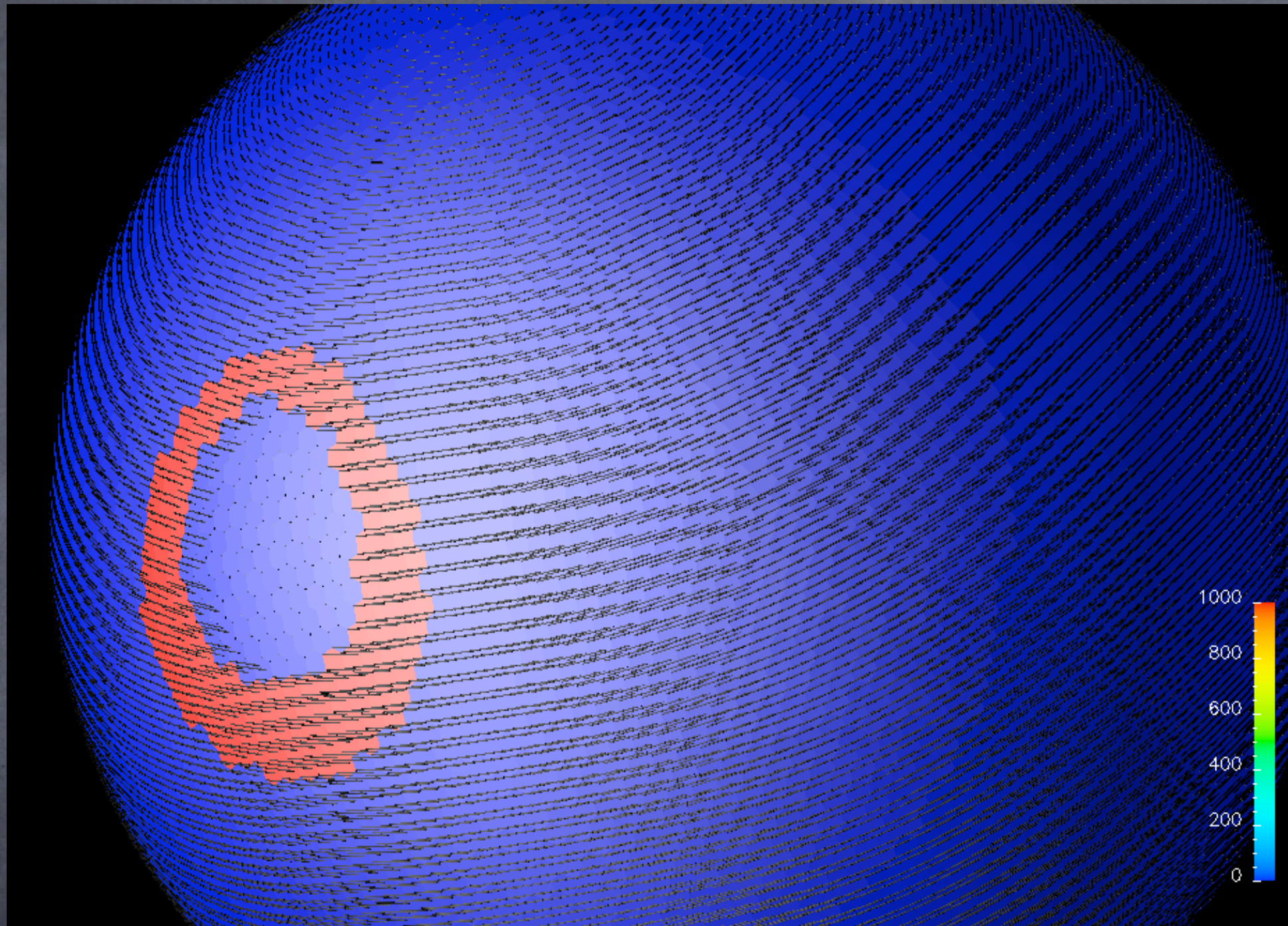
Before $t=0$ times, the flow is in geostrophic balance with a jet of 20 m/s at the equator, decaying to zero at the poles.

At $t=0$, the mountain appears instantaneously creating a large forcing to which the flow has to adjust.

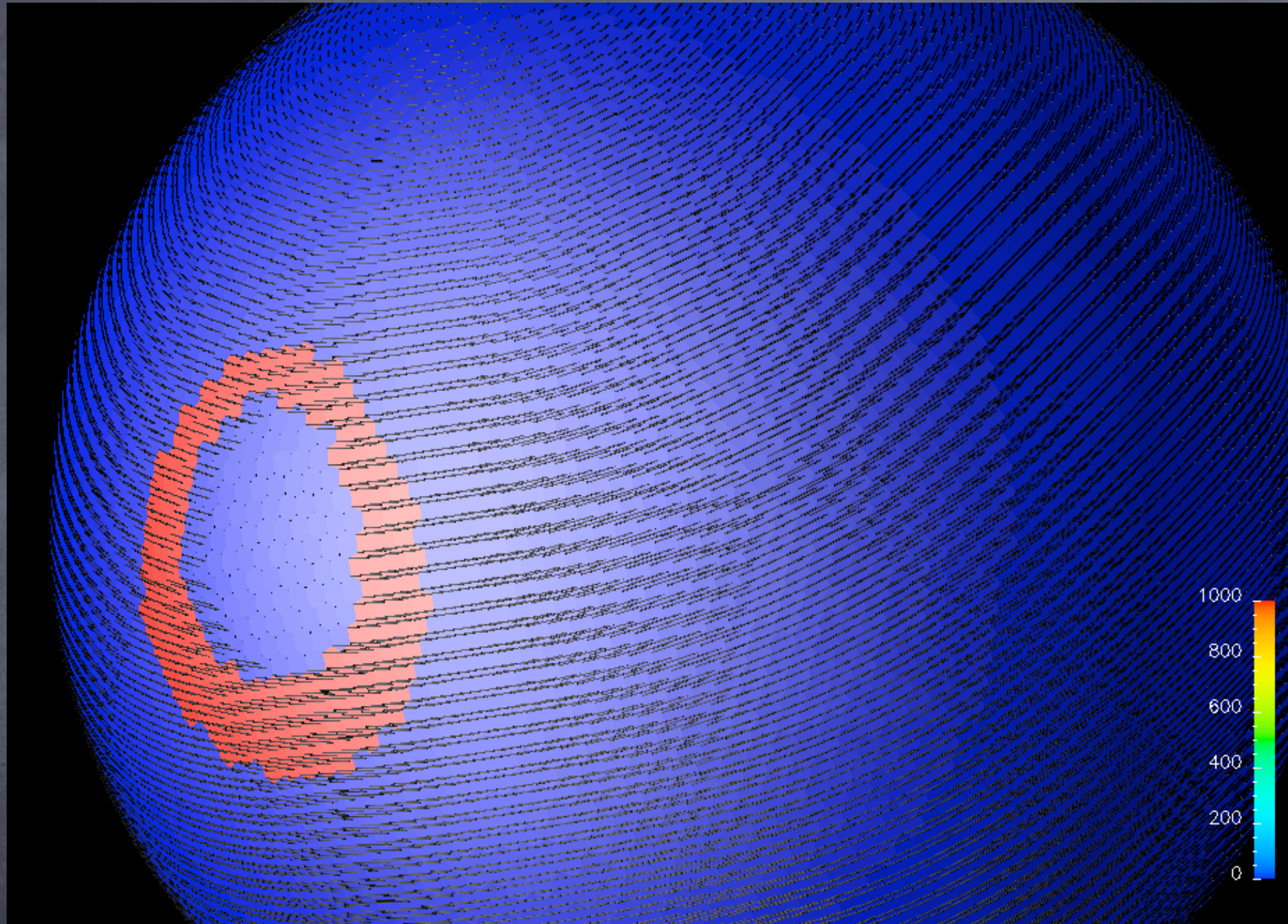


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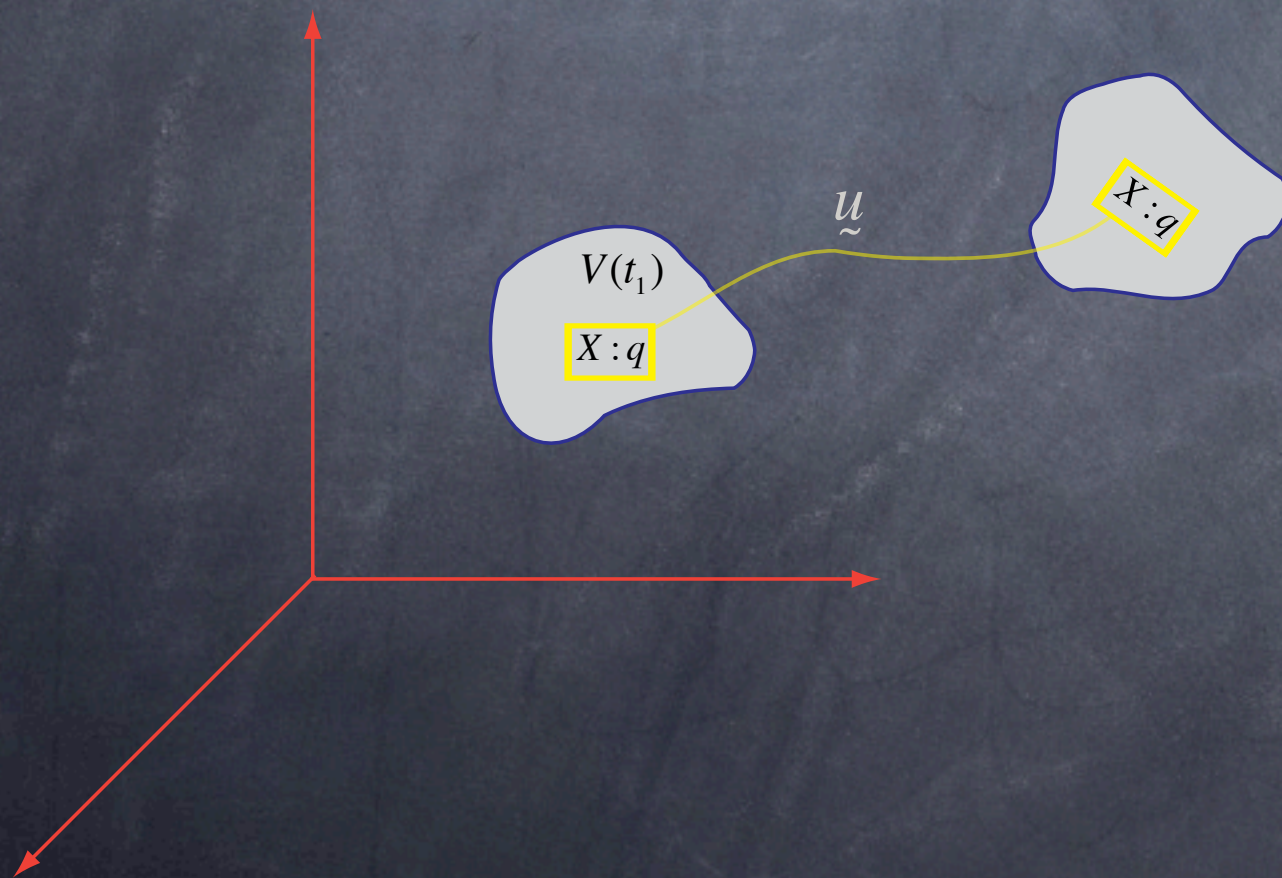
Recall that the particle tags should be invariant in time.

Also note that at $t=0$, there are only two types of labels: 0 and 1000.

By the end, there are very few locations with 1000 (the scheme is diffusive).

Transport and Monotonicity

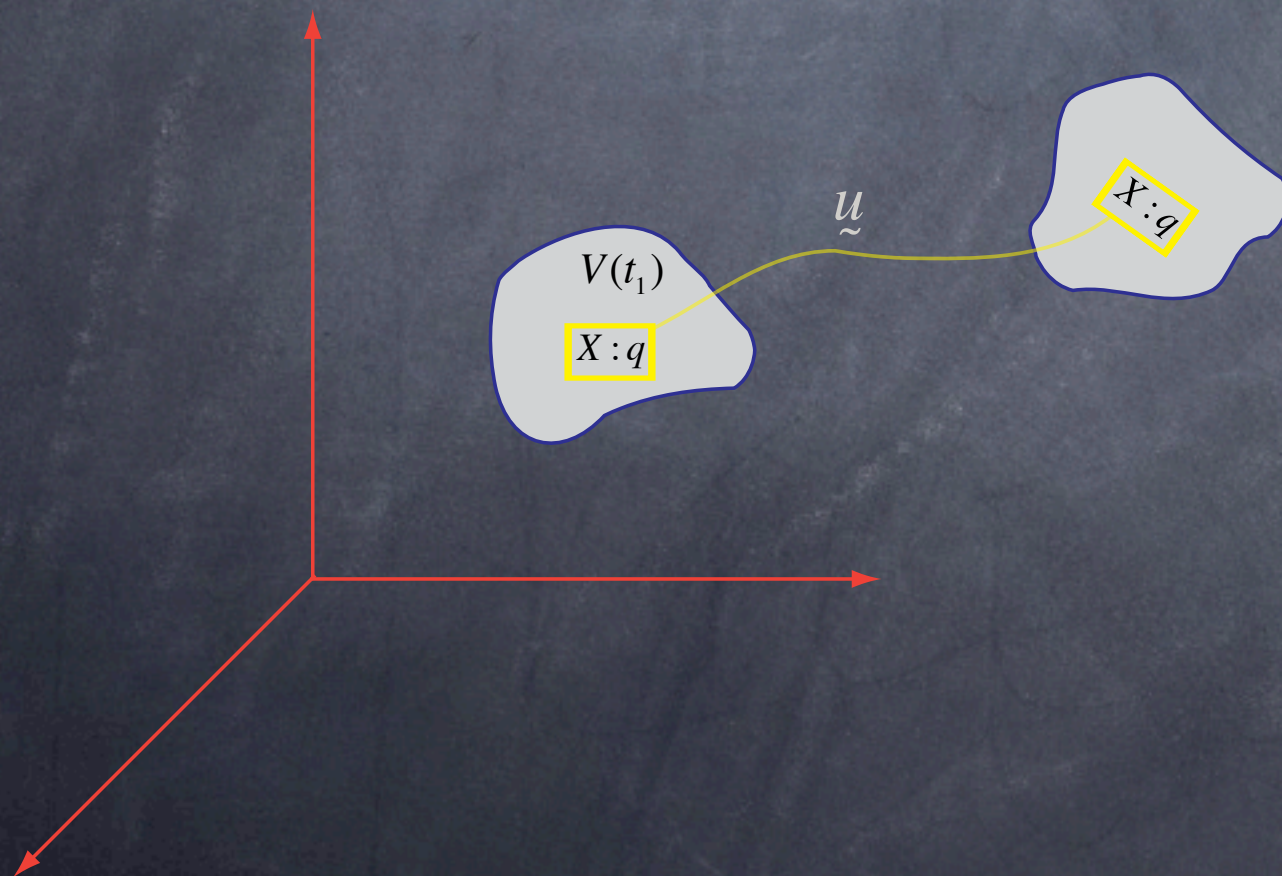
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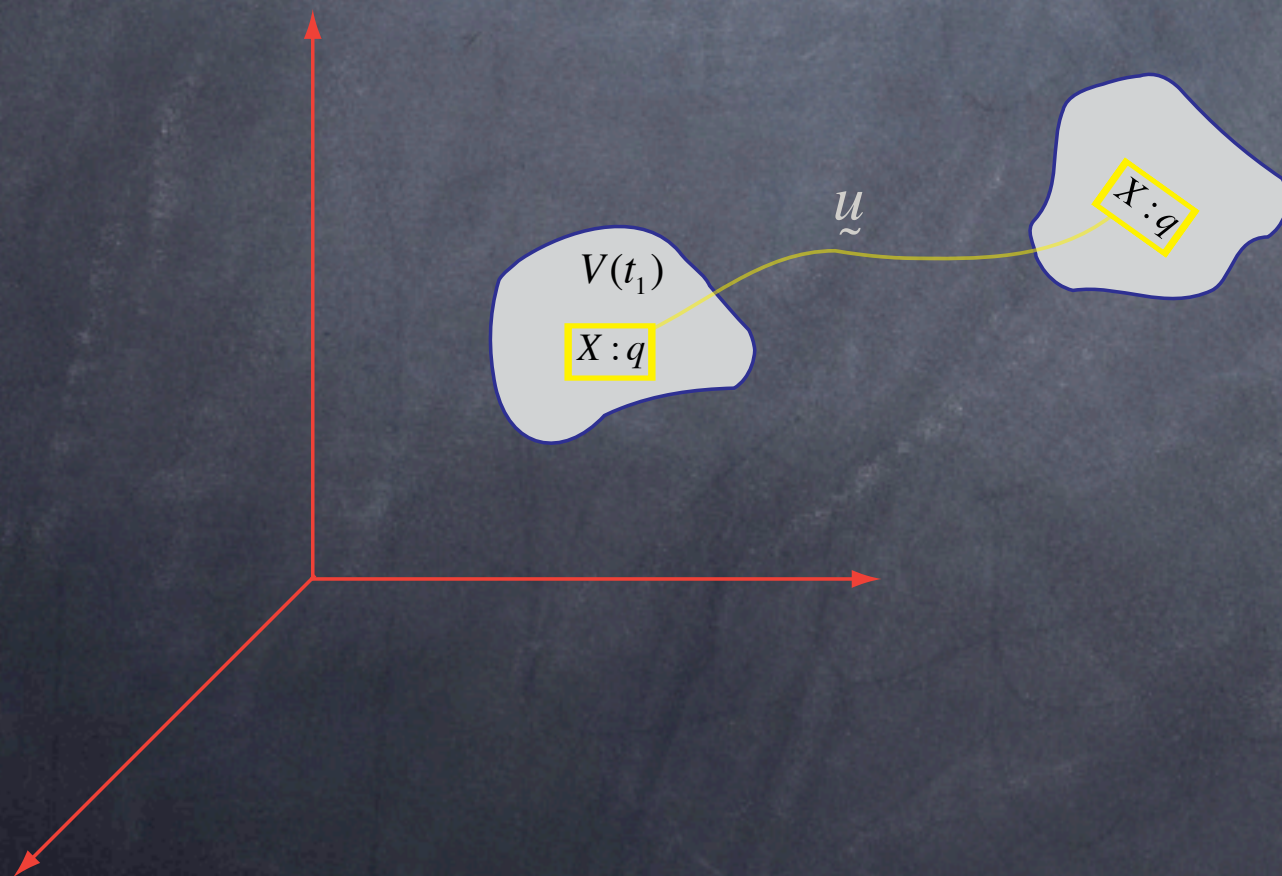
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$q_i^{n+1} = \sum_{j=1}^N \alpha_j q_j^n \quad \alpha_j \geq 0 \longleftarrow$ New values are an interpolation of old values.

$0 \leq \alpha_j \leq 1, \quad \sum_{j=1}^N \alpha_j = 1 \longleftarrow$ required for consistency



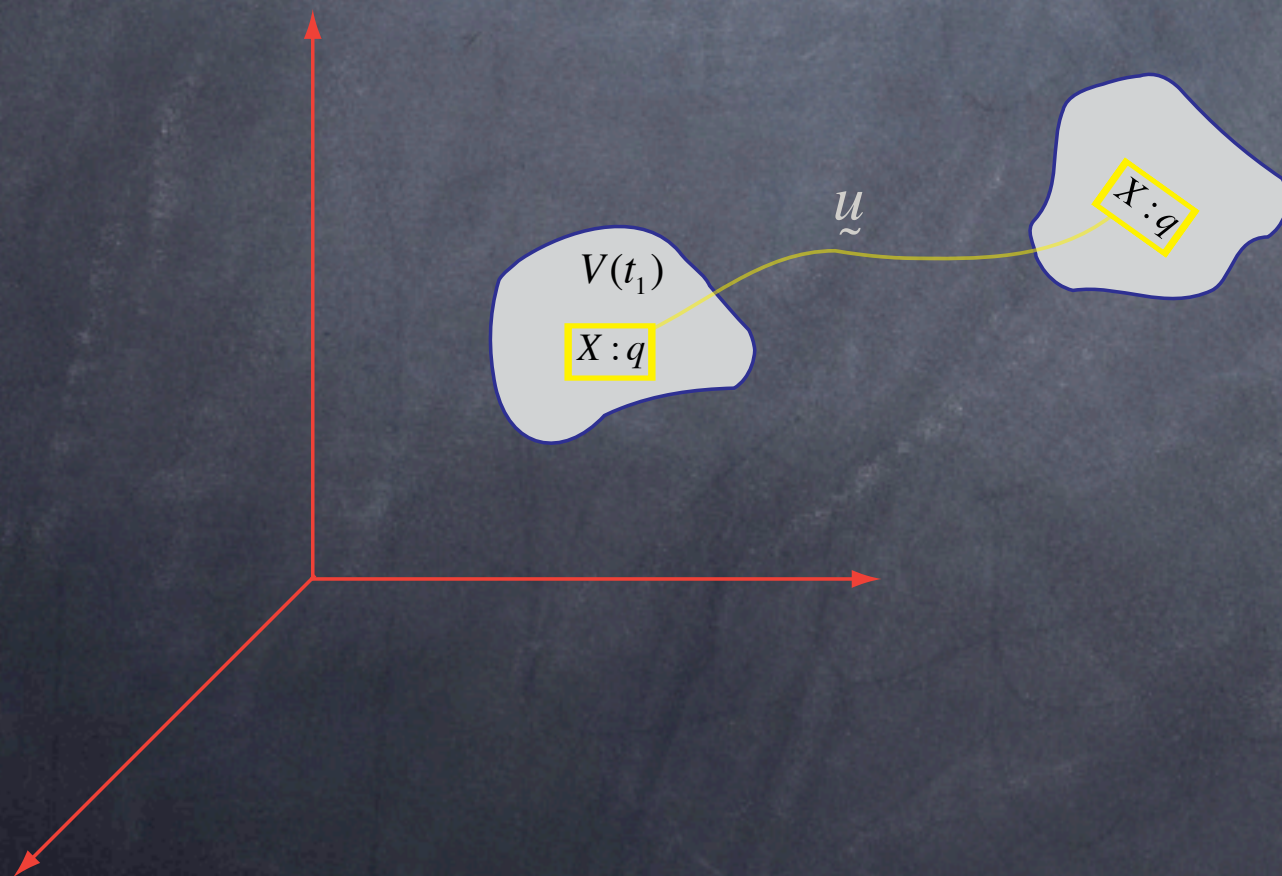
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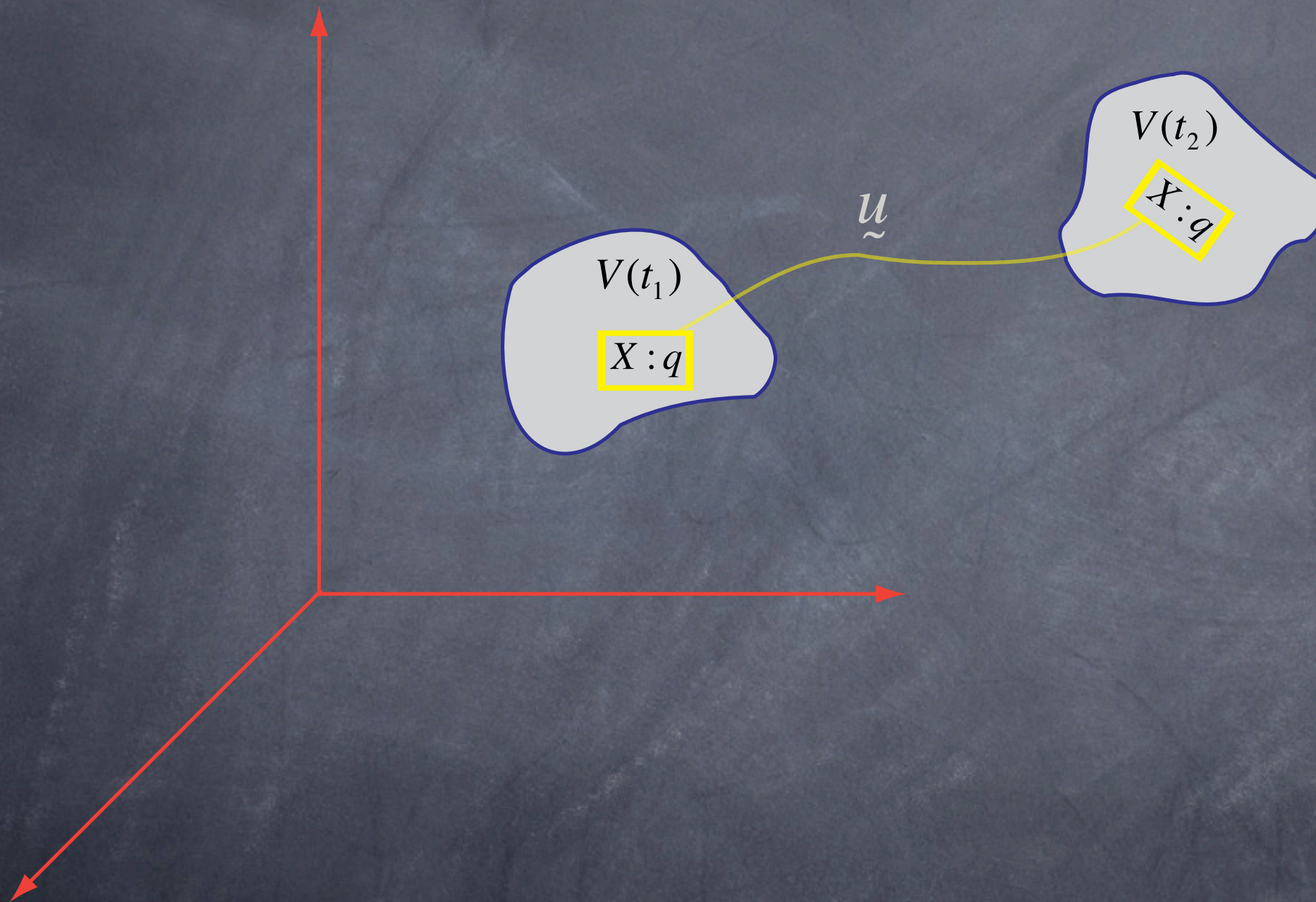
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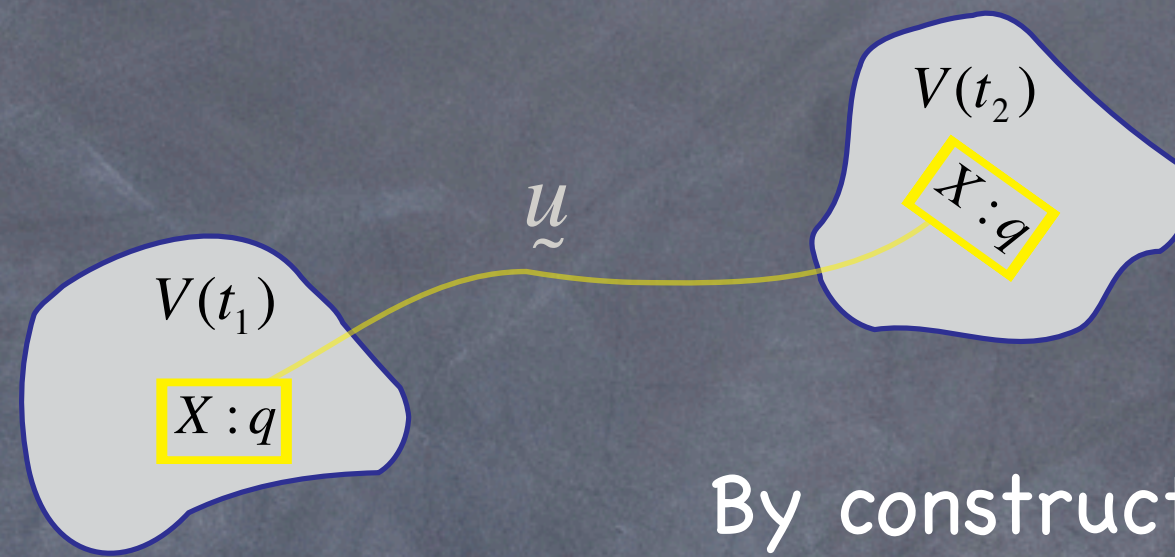
The transport conundrum

- 1) Monotonicity is a property of the continuous operator.
- 2) Godunov (1959) proved that only 1st-order accurate interpolators have the properties to guarantee monotonicity.

Why not pose the problem in the reference frame moving with the fluid?

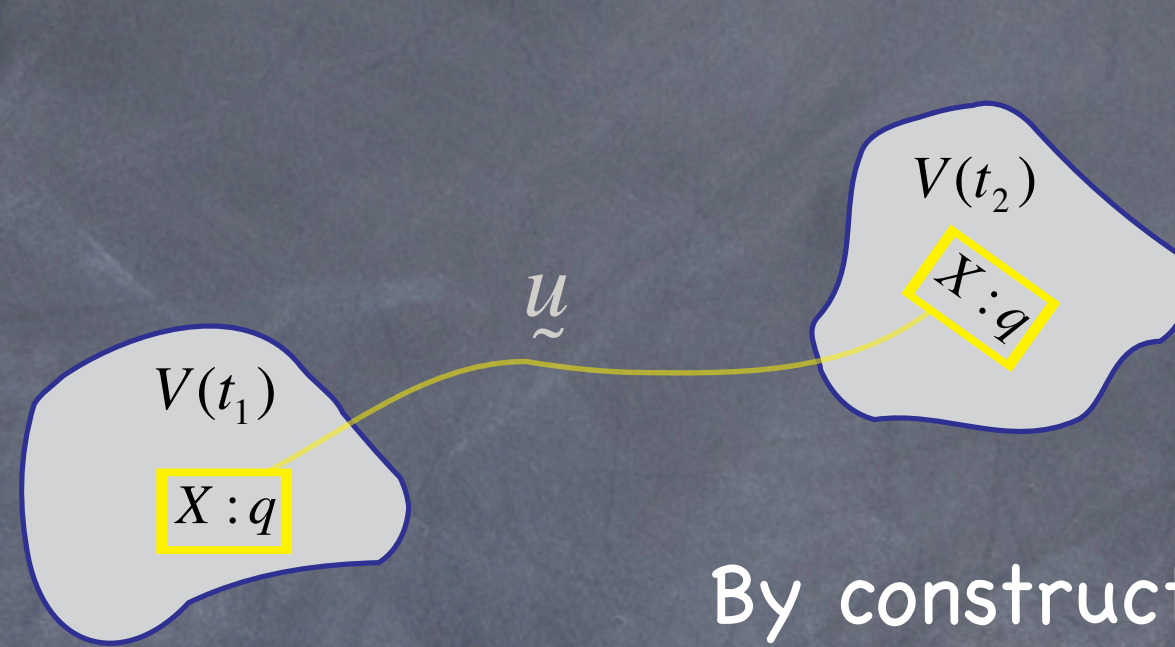


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By construction, particle tags (or regions of fluid given a single tag) remain unchanged, so the method is non-diffusive.

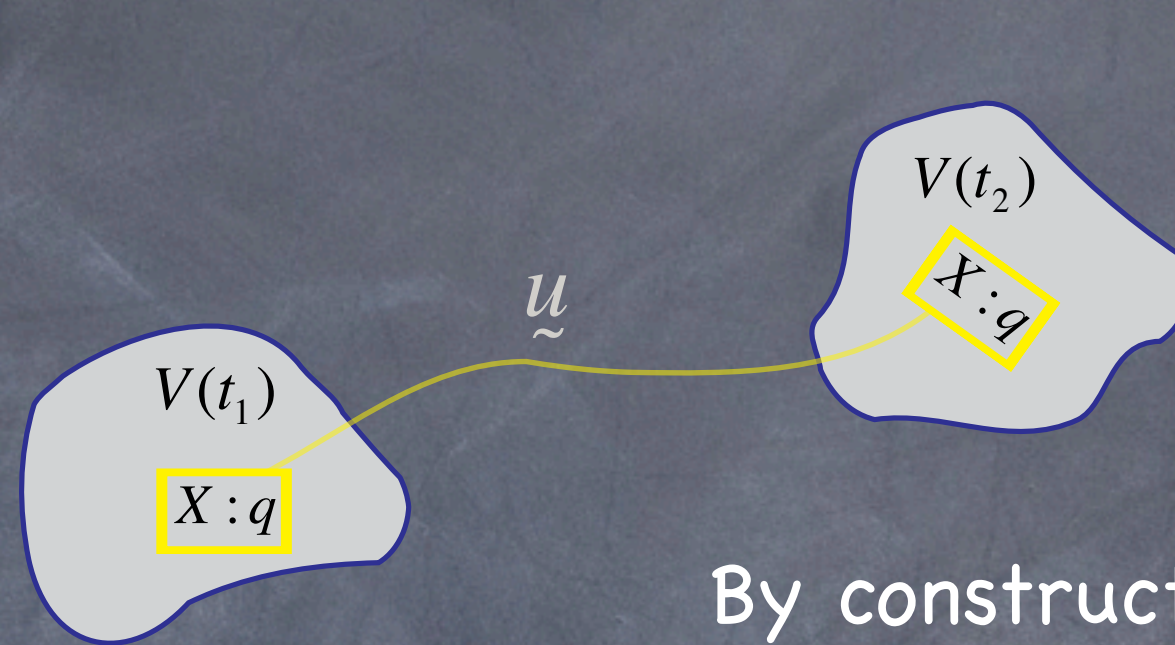
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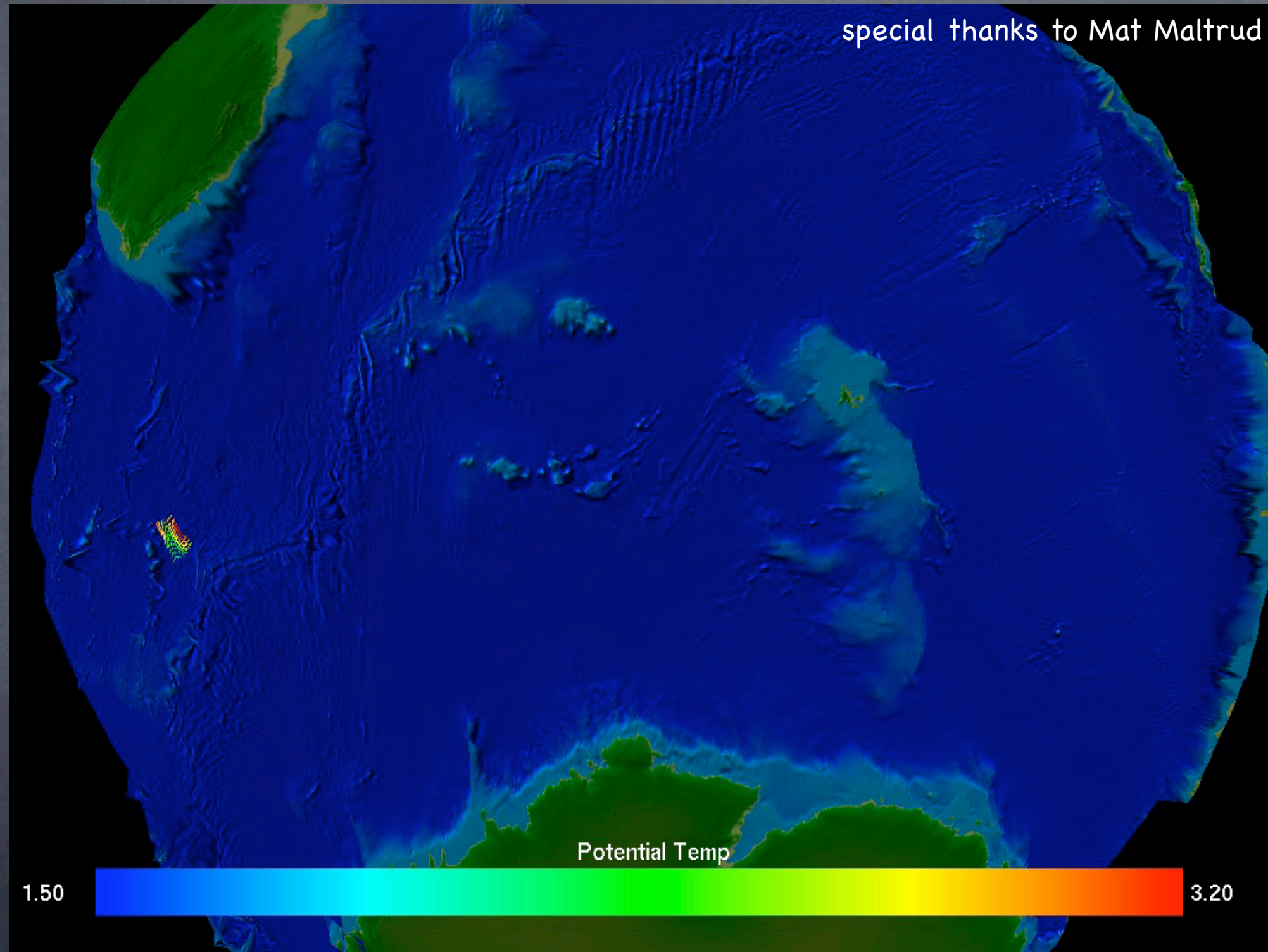
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The reason: Particles disperse rapidly, implying strong shearing/
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special thanks to Mat Maltrud

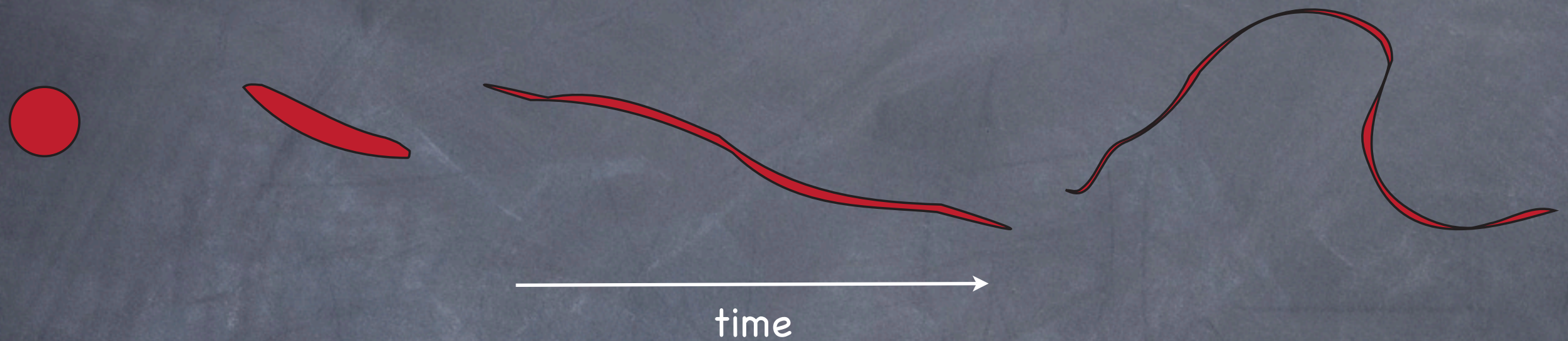
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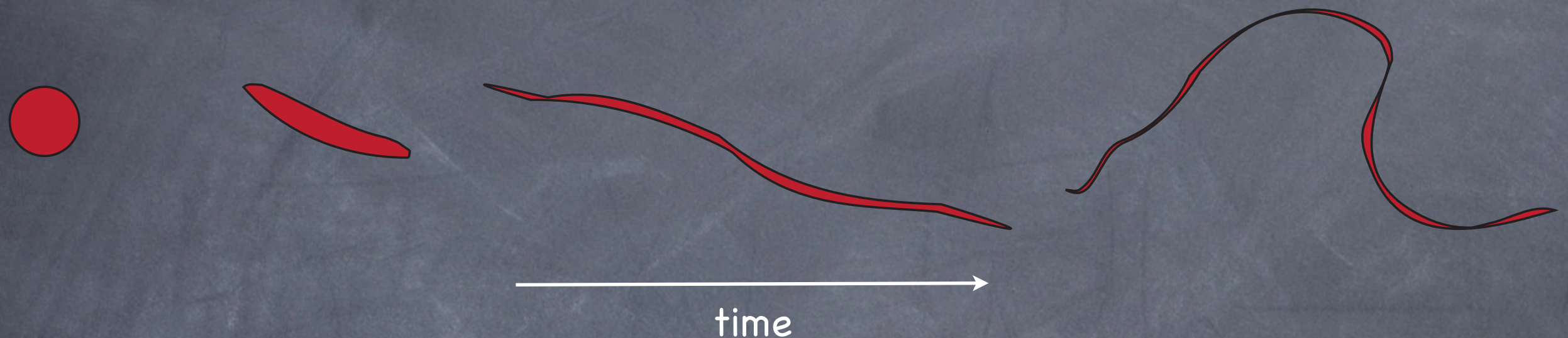


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Tracking these rapidly deforming regions in time is a huge challenge.



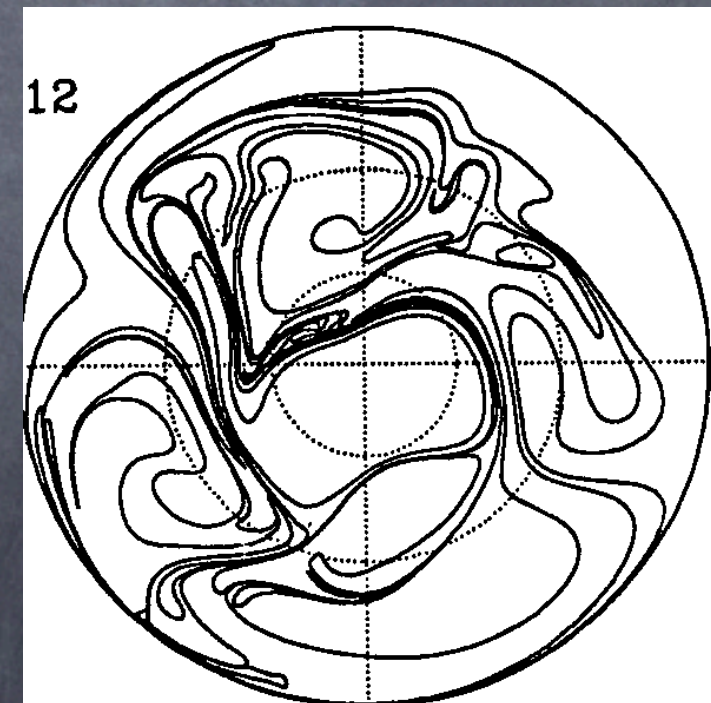
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Contour advection tracks the evolution of vortex lines, so it is a fully-Lagrangian method.

A significant amount of effort (referred to as surgery) is required to clip filaments that get too thin.

contour surgery



Waugh (1993)

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global spectral methods
spectral element methods
mesh-free finite-difference methods

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The chemistry models used in climate-mode essentially require a conservative form of tracer transport (i.e. the flux form).

That said, the advective form has been used with great success in weather prediction models using semi-Lagrangian transport.

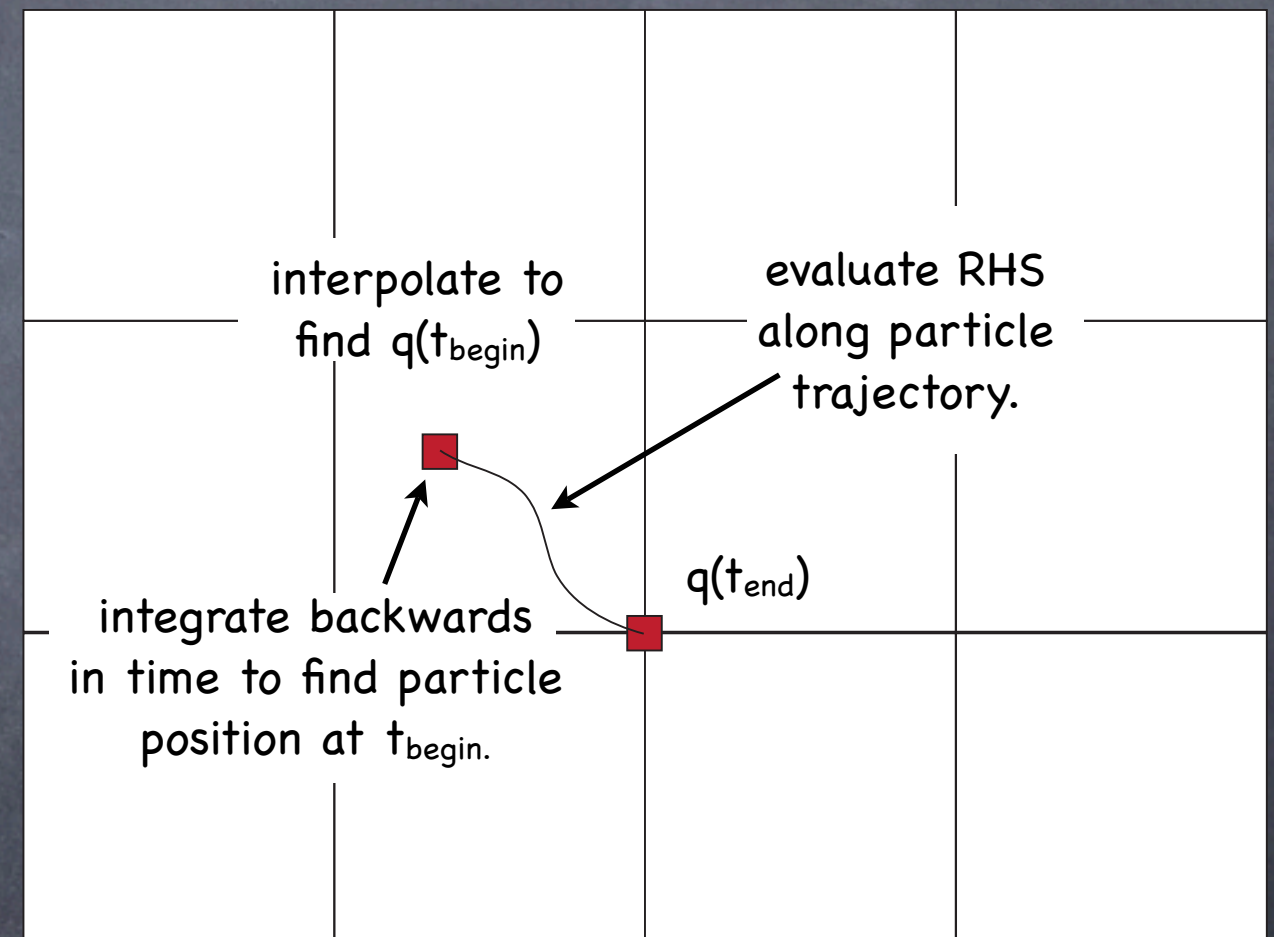
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1) start with $\frac{Dq}{Dt} = 0$.

2) integrate along a particle backward in time from t_{end} to t_{begin} , where we require the particle to “land” on the mesh at t_{end} .

3) using mesh values of q , interpolate to find the value of q at the location where the particle resided at t_{begin} .

4) set $q(t_{\text{end}}) = q(t_{\text{begin}})$



note: sources of q need to be evaluated along the particle trajectory.

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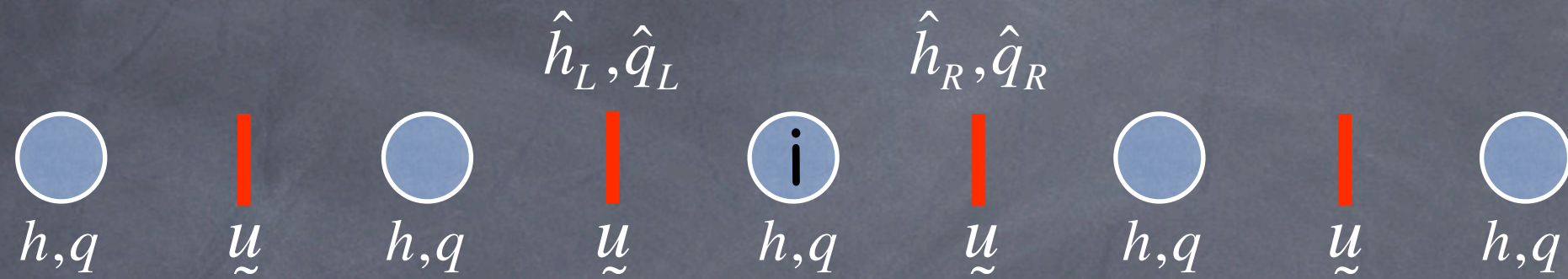
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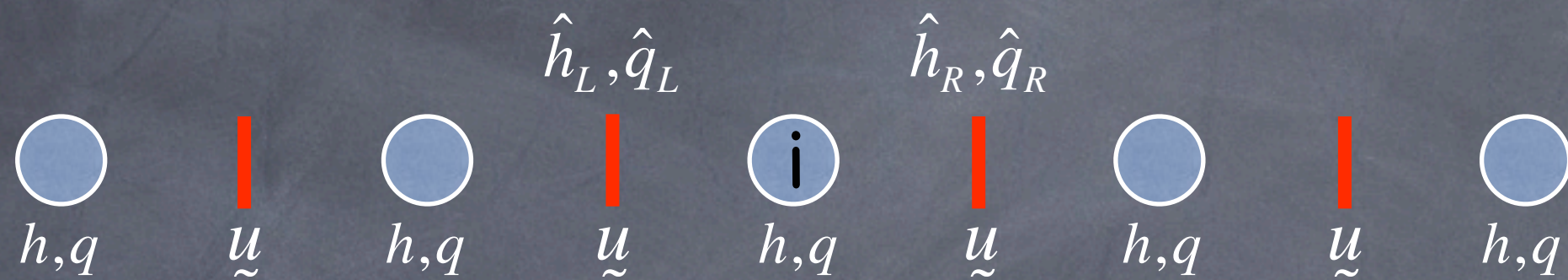
$$(hq)^{n+1} = (hq)^n - dt \left[\overline{\nabla \cdot (hq \underline{u})} \right]$$

$$q^{n+1} = \frac{(hq)^{n+1}}{h^{n+1}}$$

Spatial discretization: Start in 1D, assume \underline{u} is given.

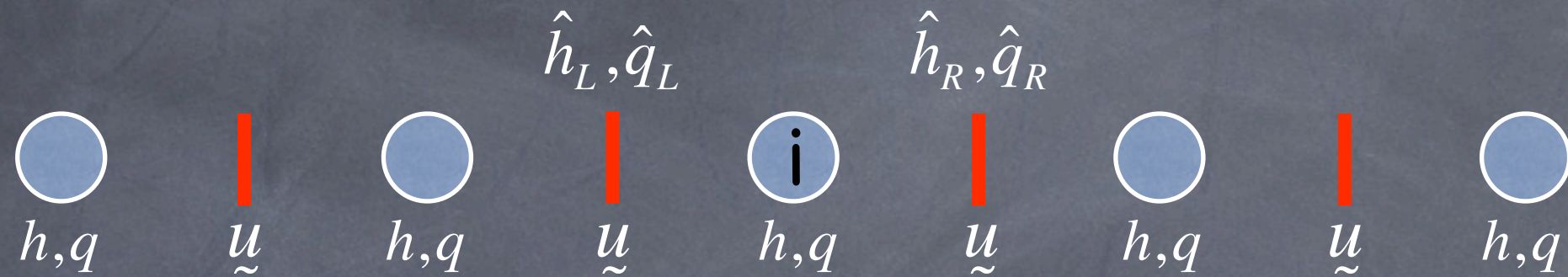


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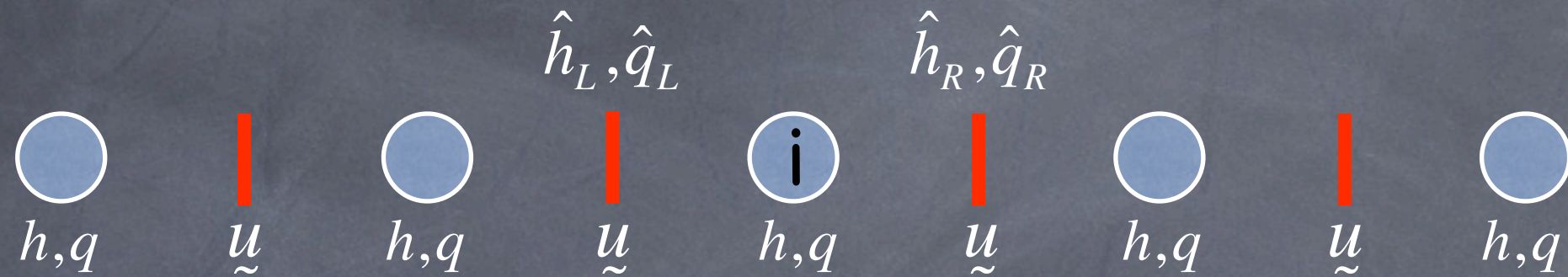
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If q is a constant, the tracer equation reduces to the mass equation. Is there a simple way to guarantee that this will be the case in our discrete system?

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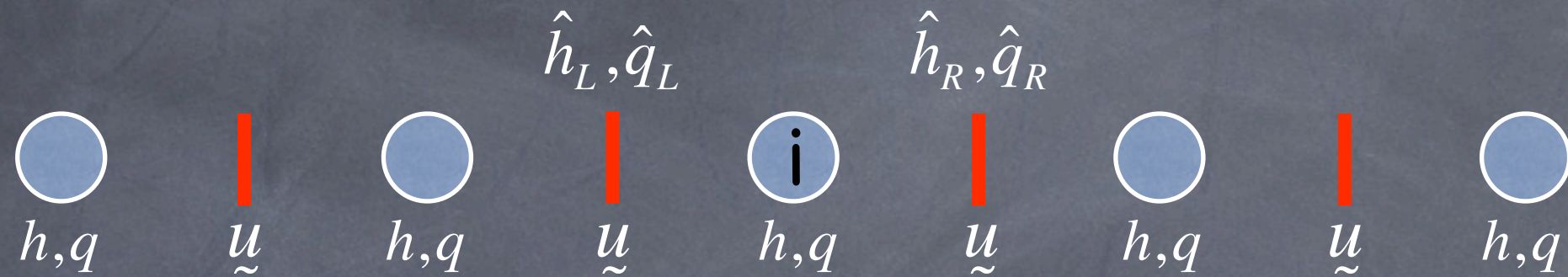
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Expressing the tracer flux as the mass flux times some \hat{q}
AND guaranteeing that \hat{q} is an interpolation of its neighbors
(i.e. \hat{q} is bounded by neighbor data) is sufficient to ensure that a
constant q remains constant and reduces to the mass equation.

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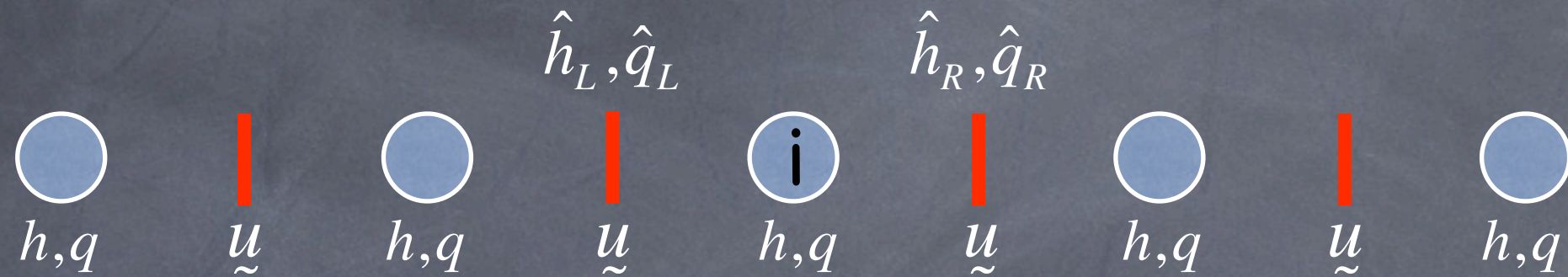


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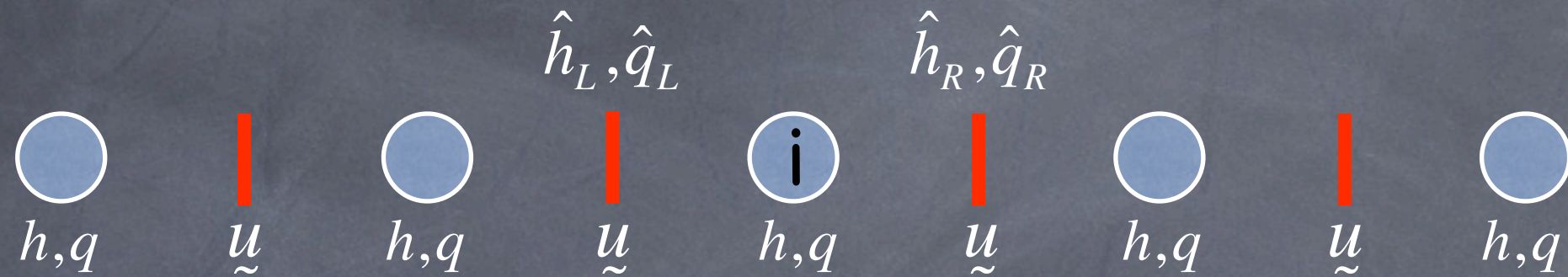
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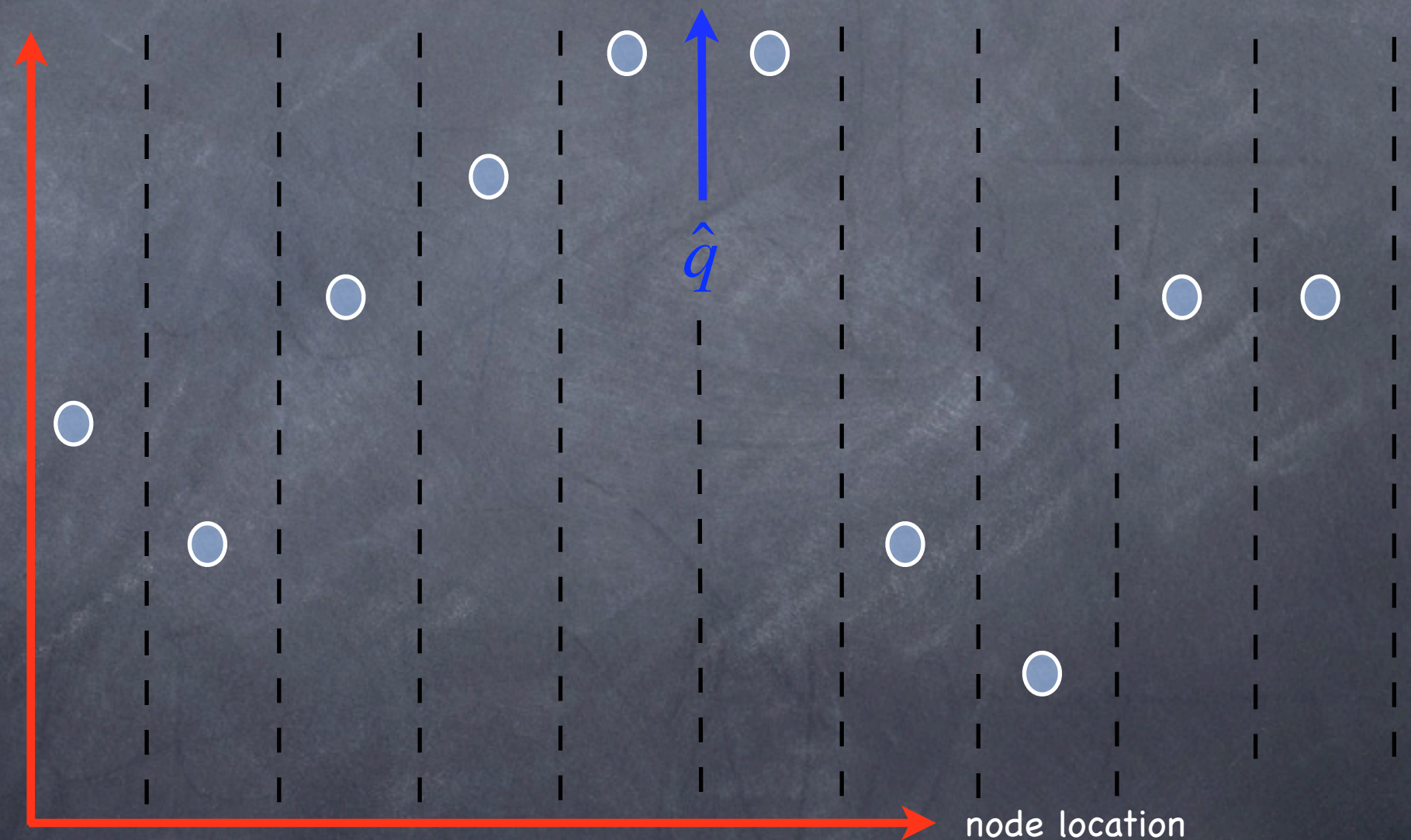
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- 1) What is \hat{h} ?
- 2) What is \hat{q} ?

Determining \hat{q} : High-order interpolation

We have our data defined at our nodes, our task is to determine \hat{q} at the interfaces.

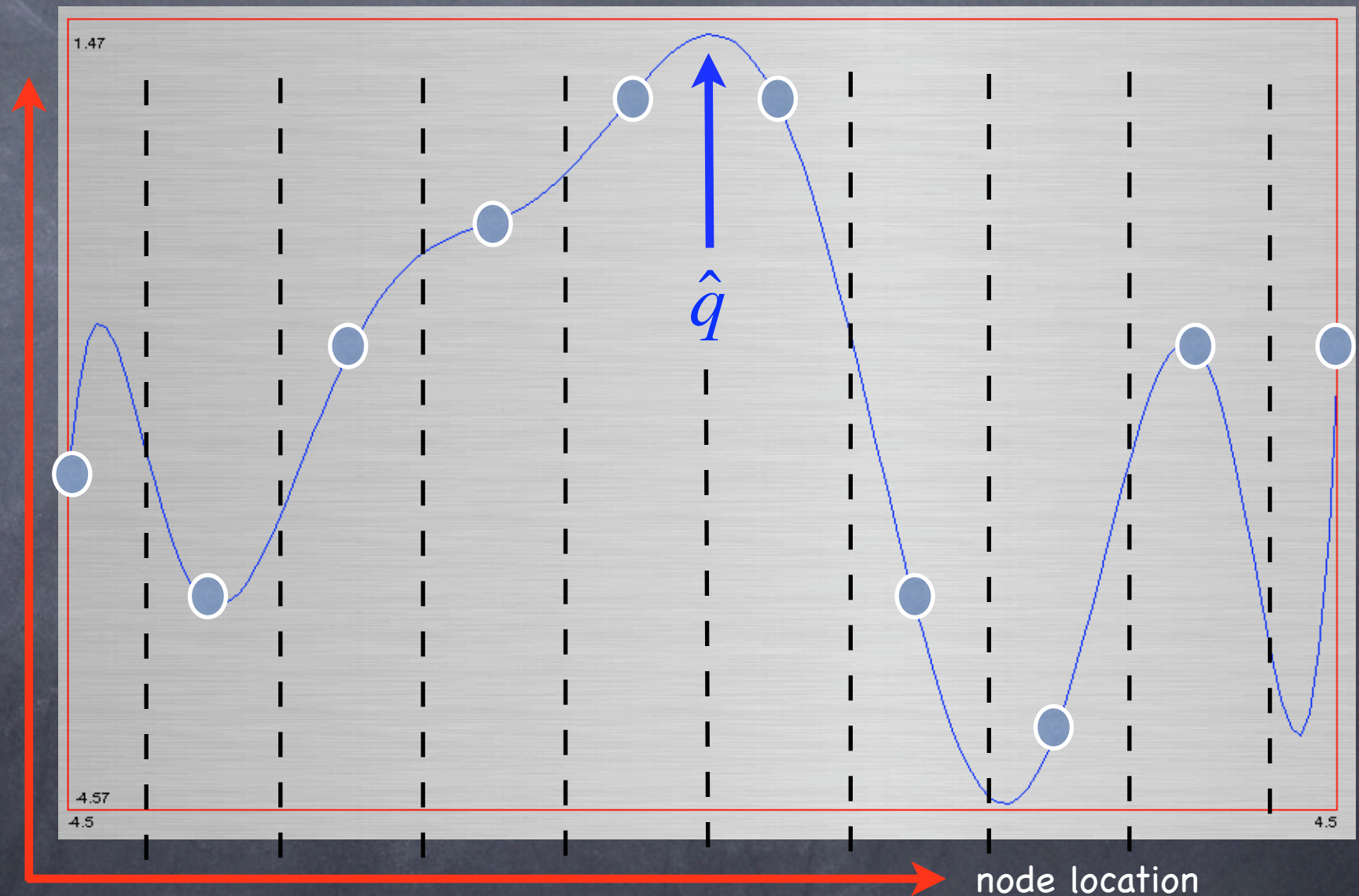
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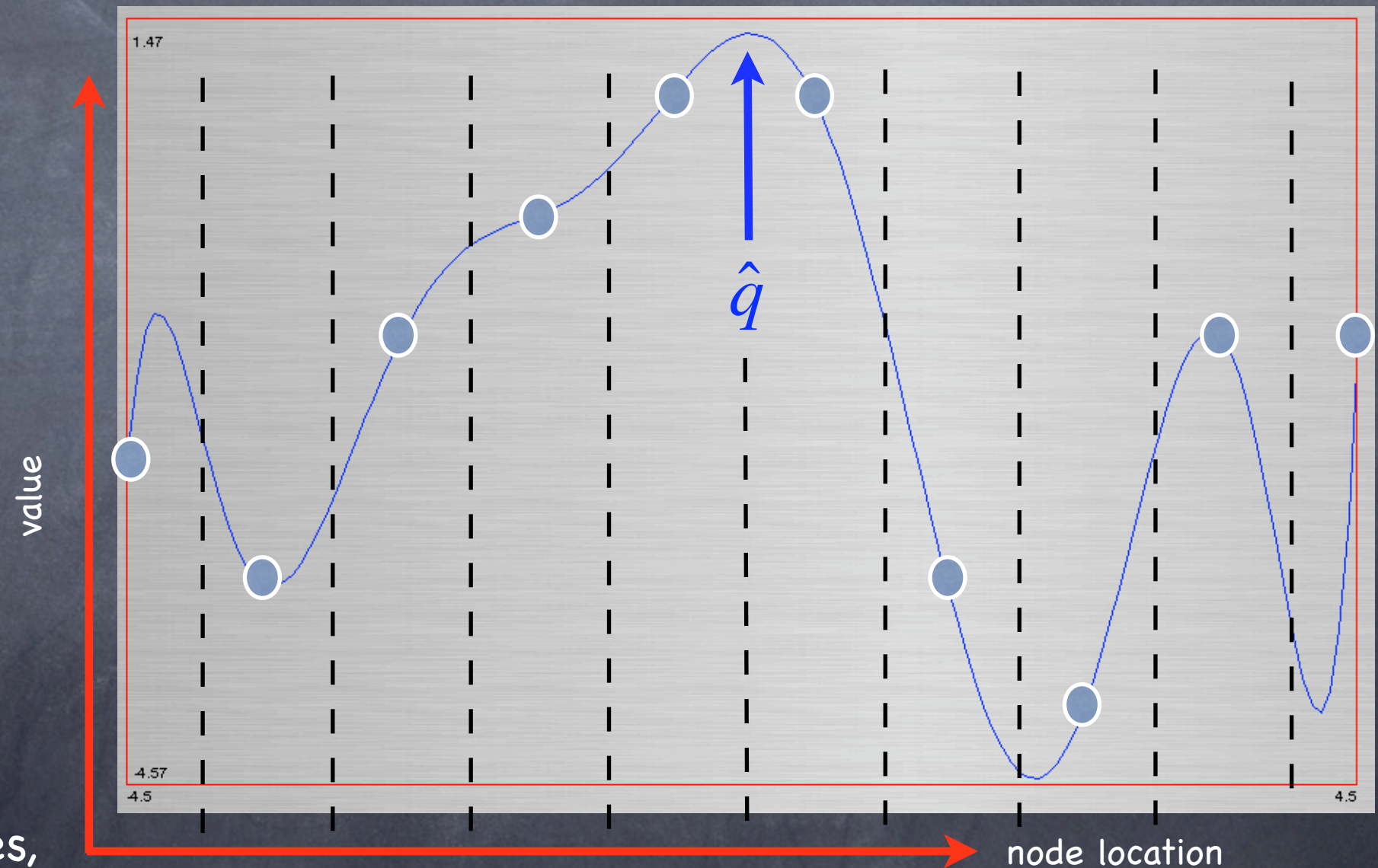
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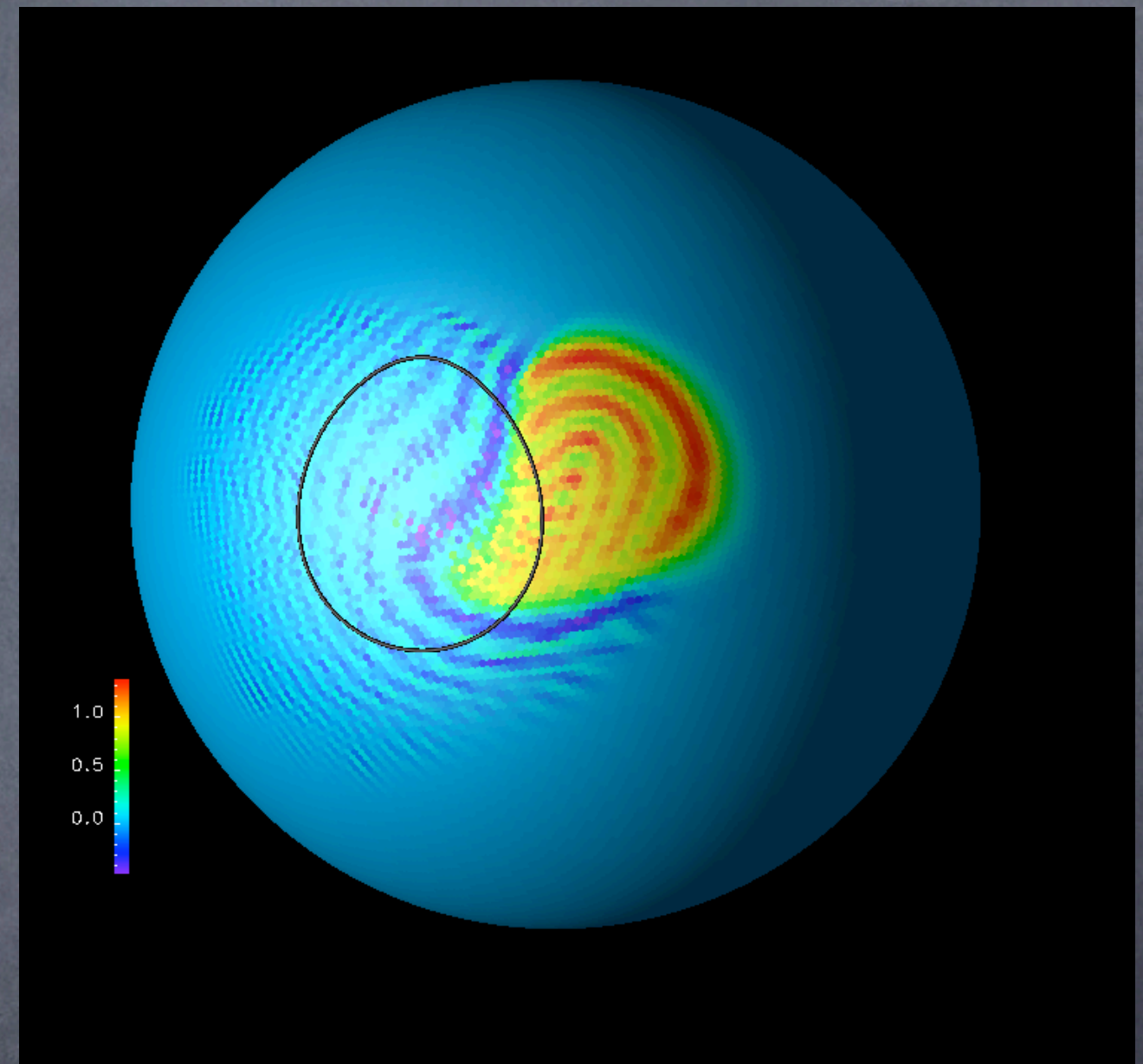
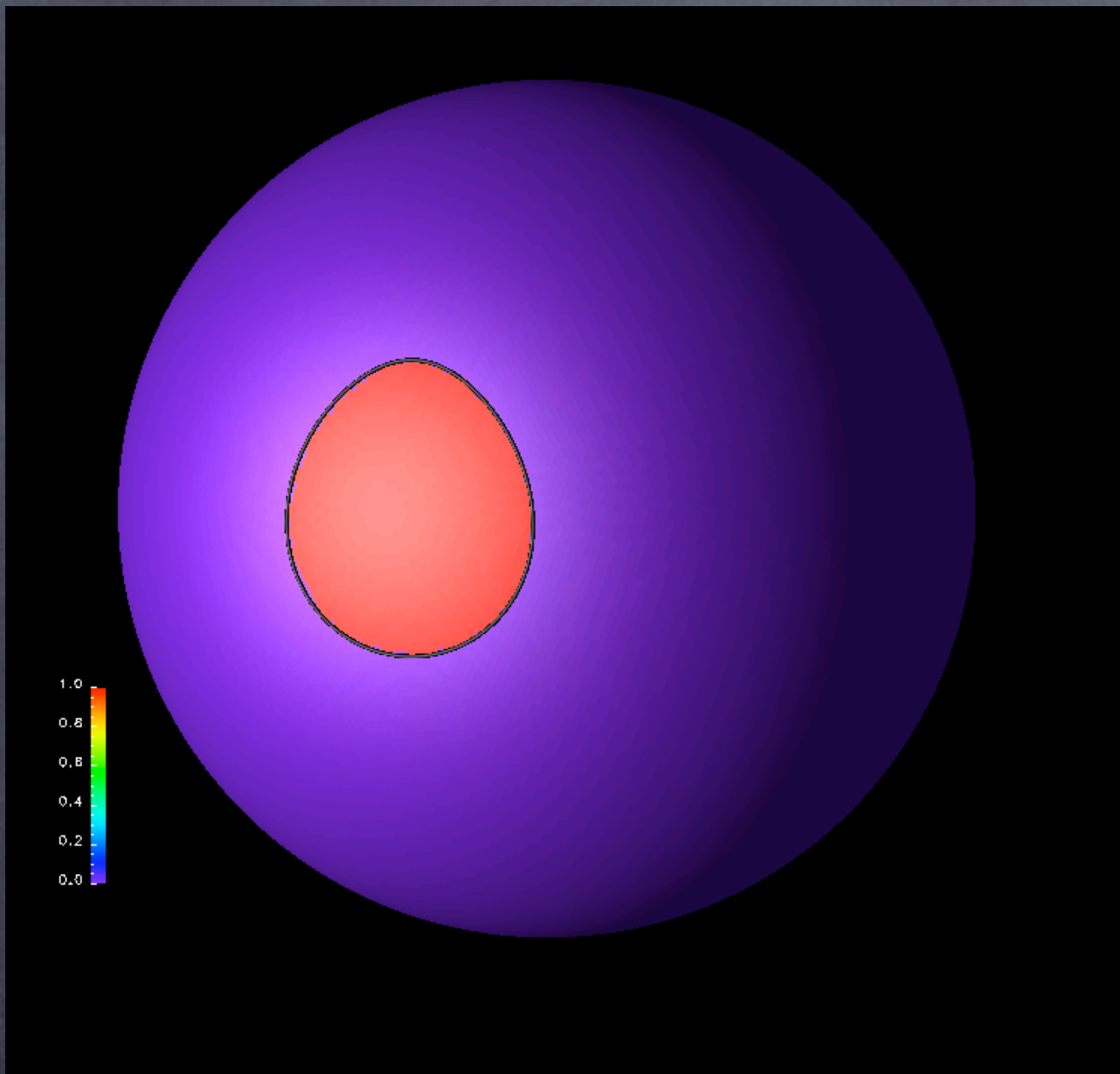
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Assessment

- 1) This is a very accurate reconstruction (9th order, in fact).
- 2) The reconstructed \hat{q} is "out of bounds" in that it overshoots and undershoots all of the mesh data.
- 3) These over/under shoots can, in some cases, contaminate the simulation.



An example of impact of under/over shoots.

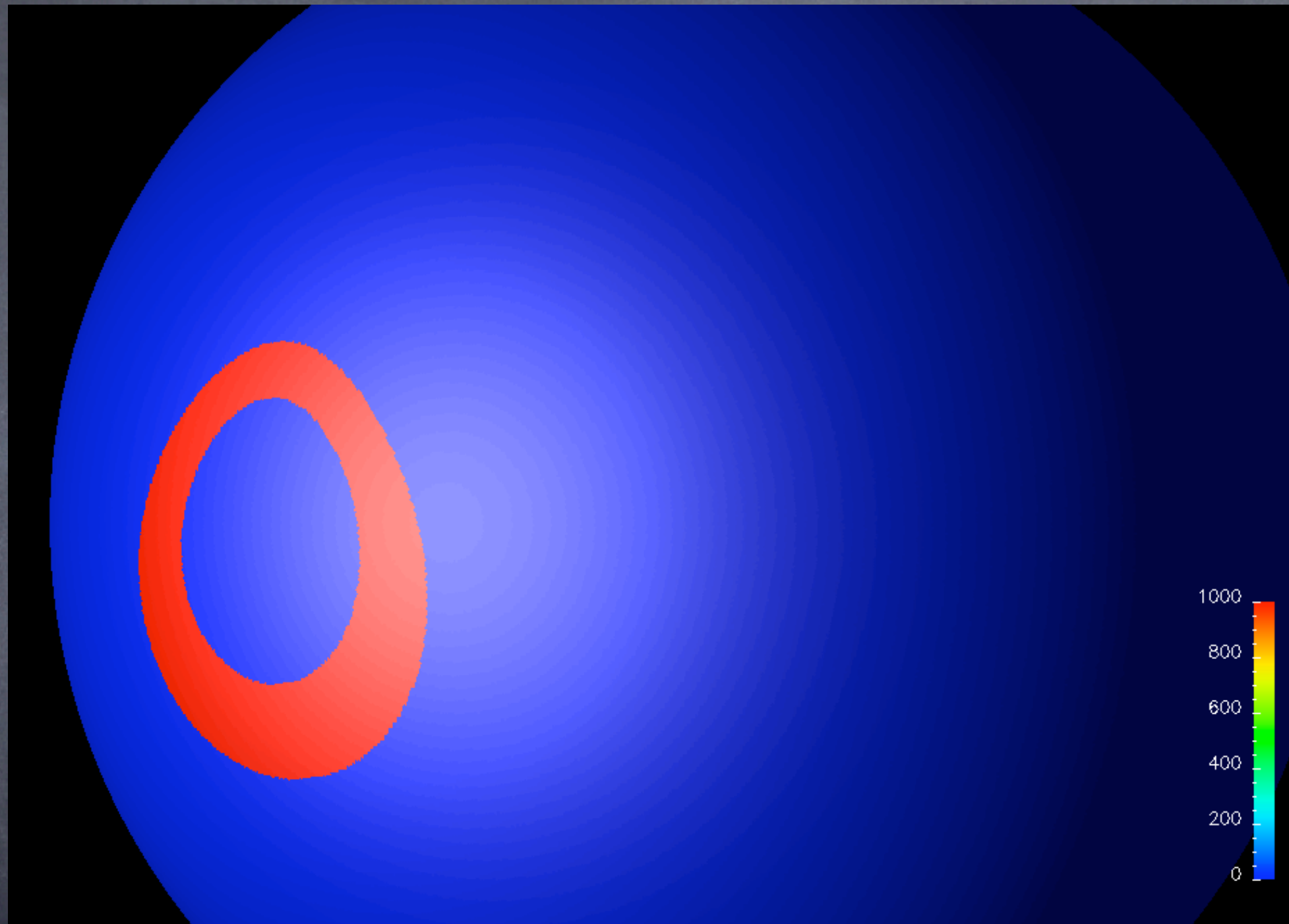


Example of dispersion:

Note: overshoots are permitted (more on this below).

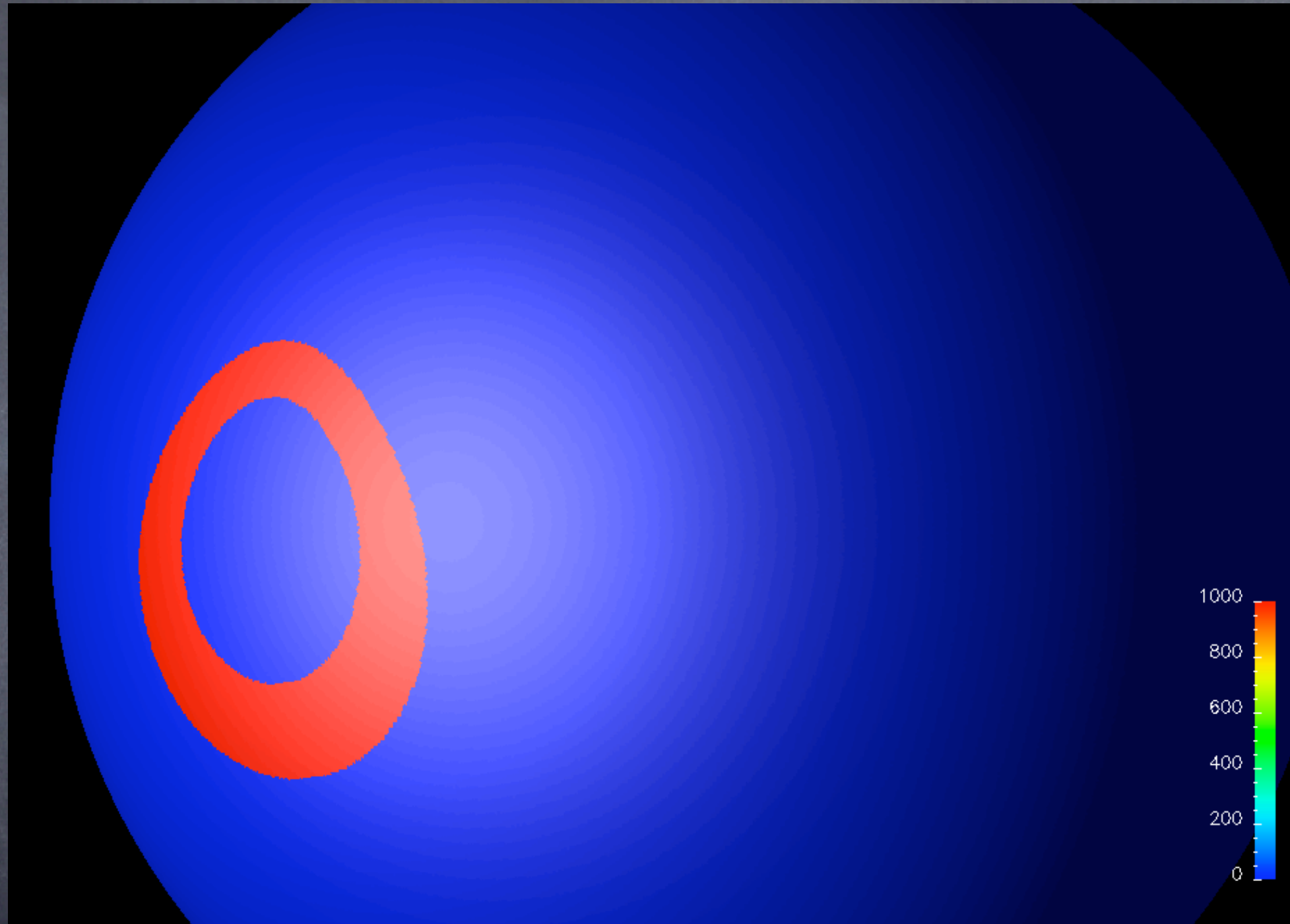
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Whether or not over/under shoots are acceptable is problem dependent. For example, a slight overshoot on CO_2 concentration is likely to be benign, while an undershoot leading to negative specific humidity will cause havoc.

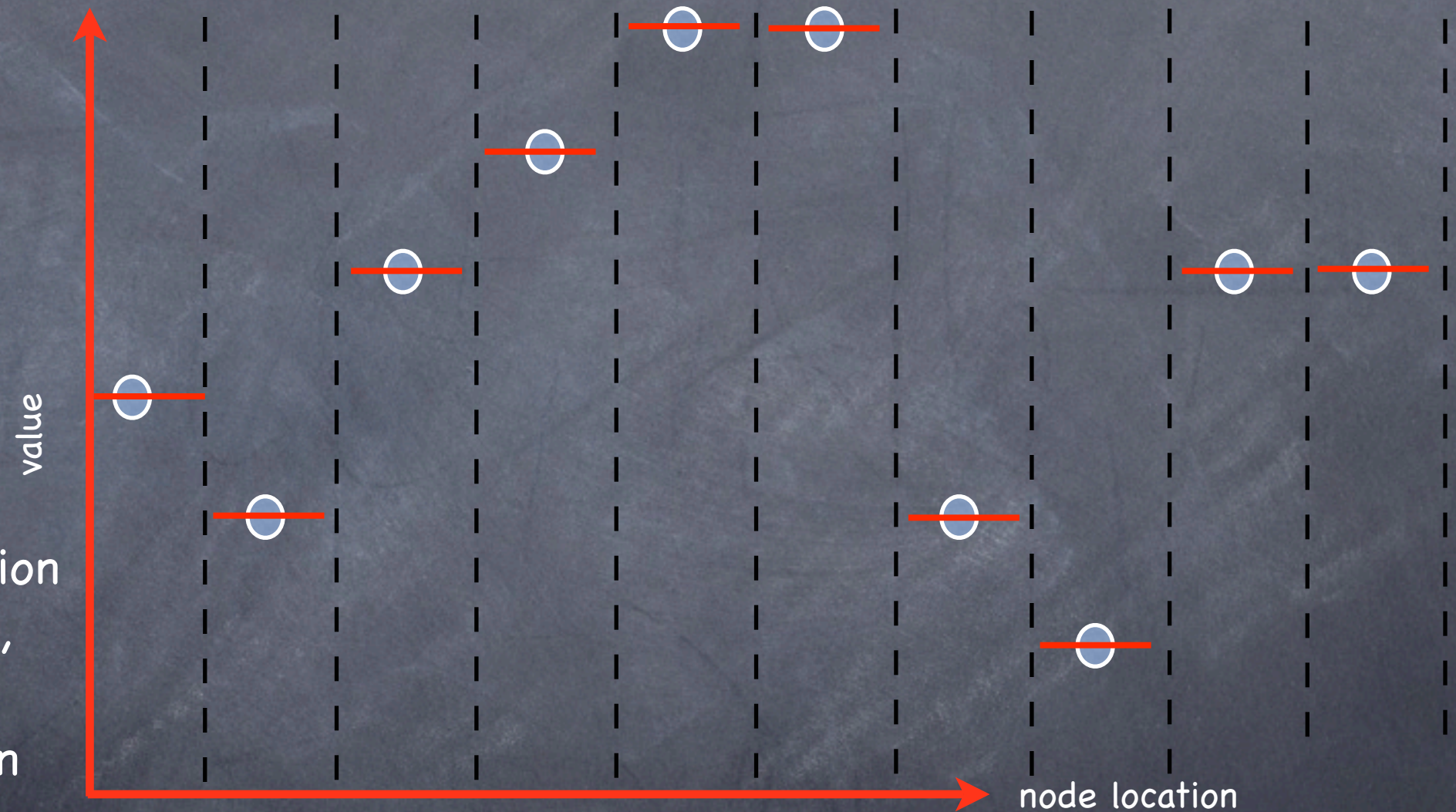
Determining \hat{q} : Low-order interpolation

→ assume a constant velocity from left to right

1) Assume a piece-wise constant reconstruction.

2) Recognize that the transport is from left to right and set \hat{q} to its **upstream** neighbor.

3) Since the reconstruction is only 1st order accurate, the leading truncation error is $(\Delta x)^2$ resulting in a highly diffusive scheme.

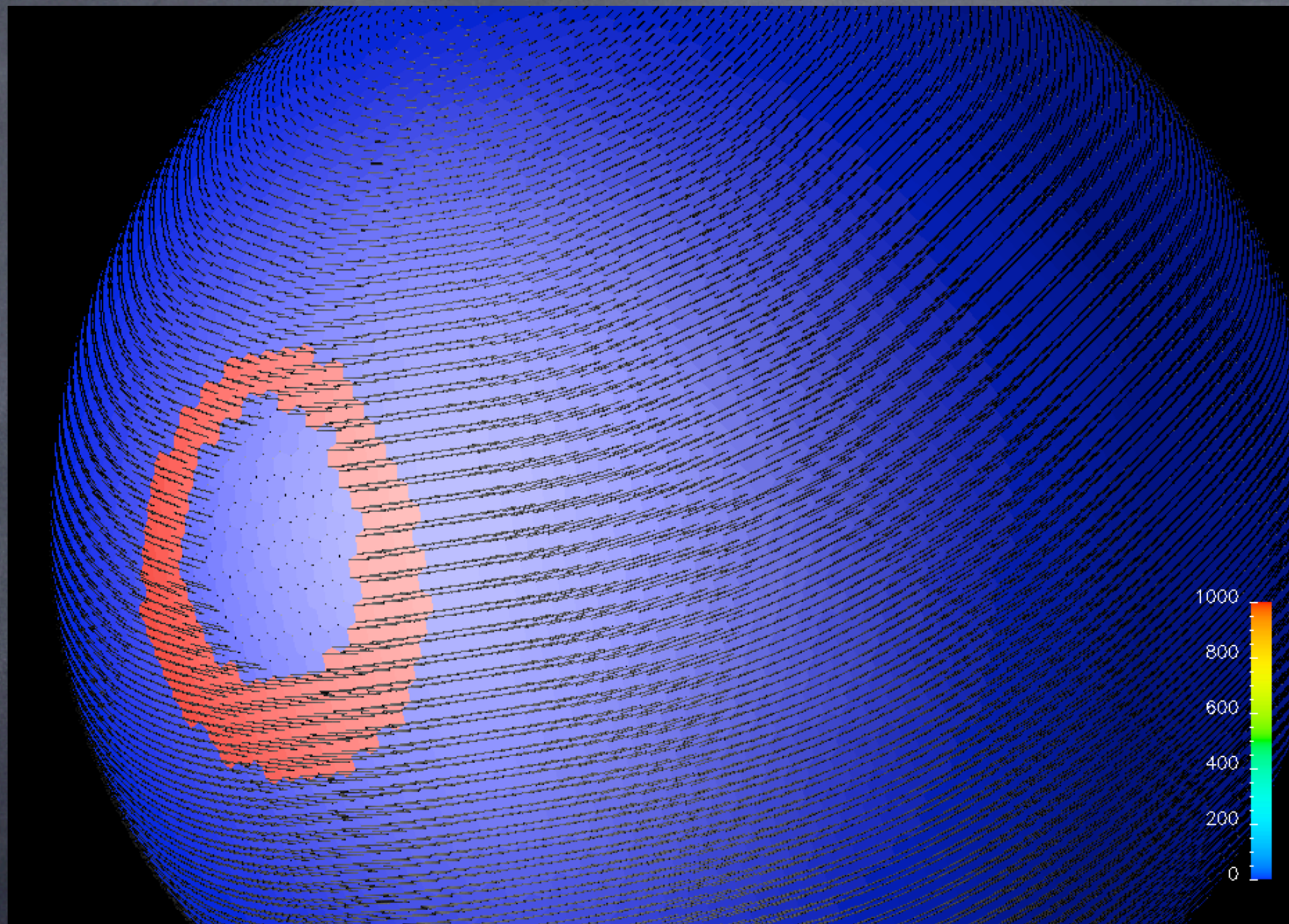


$$q_i^{n+1} = q_i^n + u \cdot dt [q_{i-1}^n - q_i^n]$$

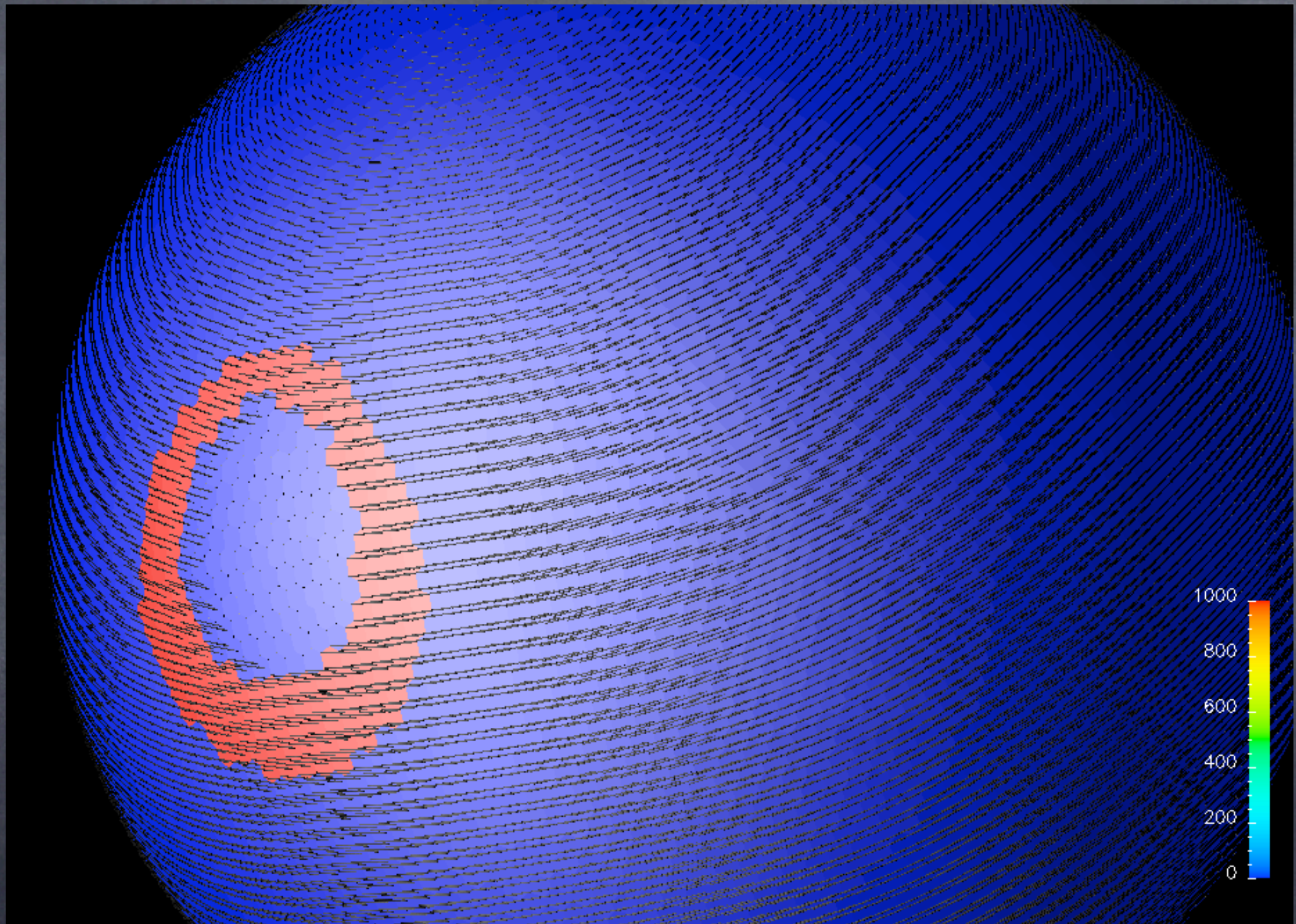
Satisfies Godunov's Theorem for $u \cdot dt \leq 1$

Example of diffusion: transport is monotone.

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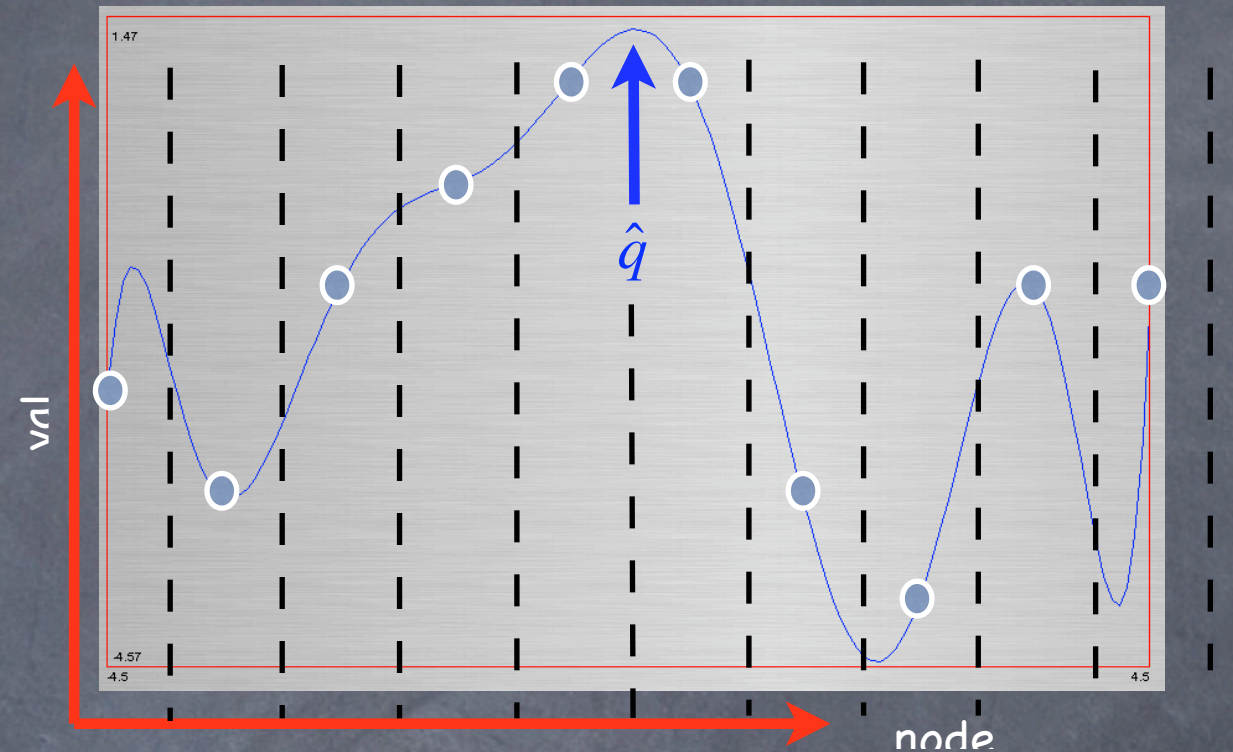


The excessive smoothing significantly degrades the quality of the simulation.

So we are left with a Goldilocks search

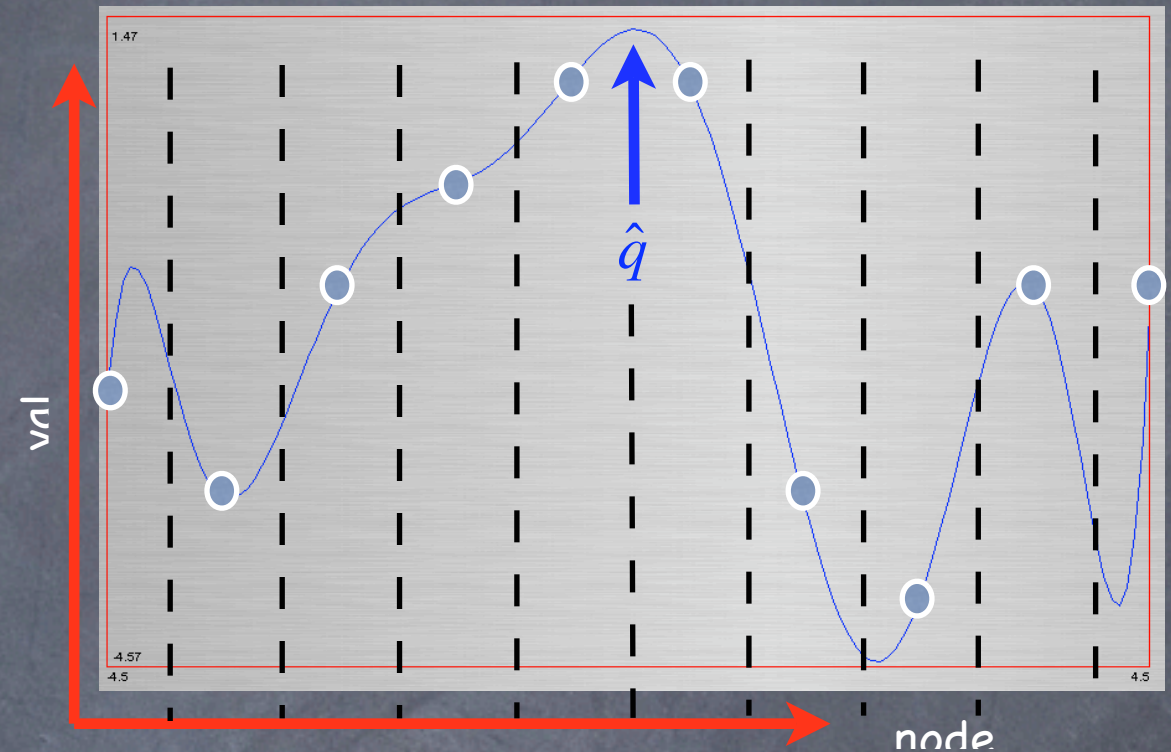
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This \hat{q} is too hard.

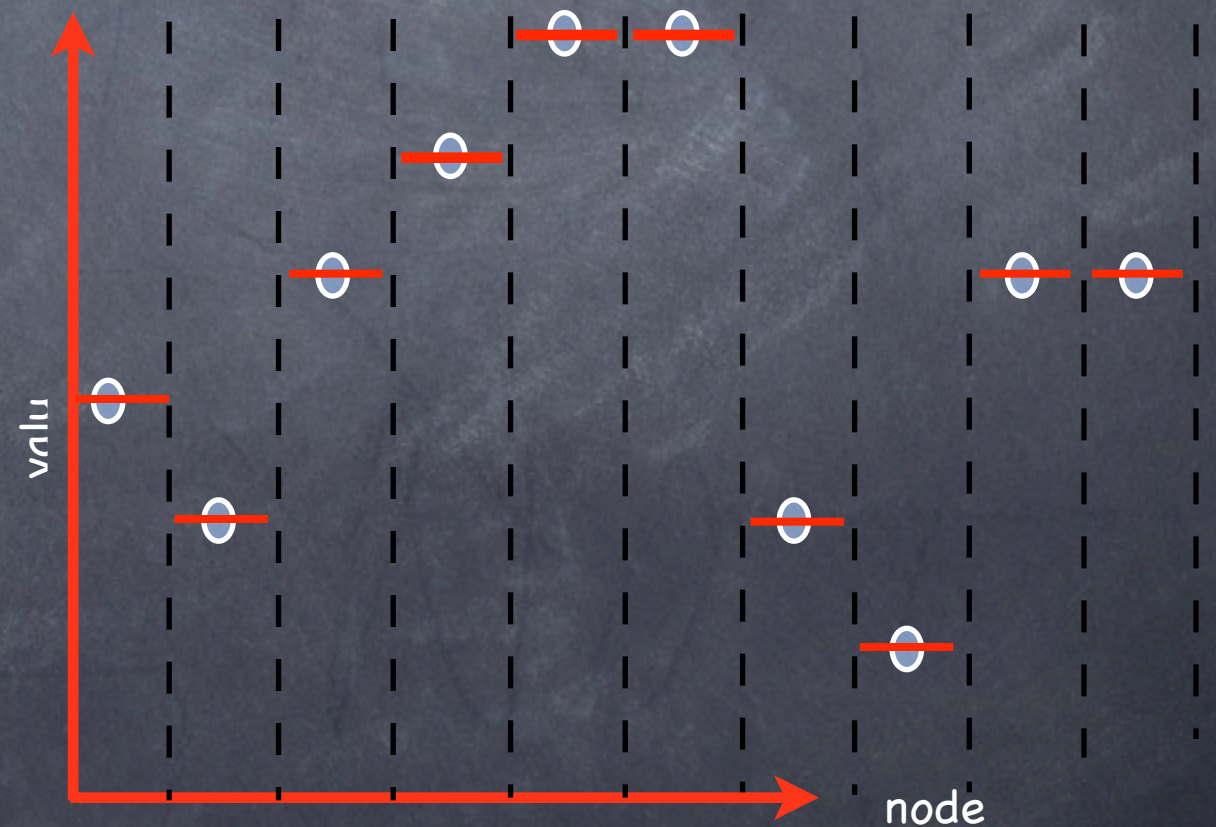


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This \hat{q} is too soft.



.... but (according to the literature) all of these \hat{q} are just right ...

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The point here is twofold:

- 1) The appropriate transport scheme is problem specific.
- 2) A tremendous amount of effort has been given to the topic of transport.

We can broadly think of schemes in one of two ways: the scheme either **limits the flux** or the scheme **limits the reconstruction**.

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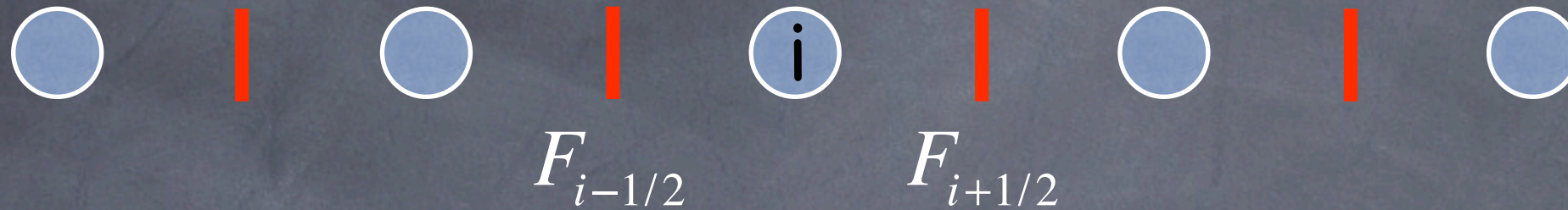
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In either case, the attempt is to modify \hat{q} in such a way as to minimize the diffusivity, maximize the formal accuracy and guarantee something about the bounds on the resulting tracer distribution.

The “guarantees” generally all into one of three categories:

- 1) monotone (as defined above)
- 2) total variation diminishing (variance between adjacent nodes reduces in time).
- 3) positive definite (just keep it above zero!).

Approach #1: Limiting the Flux



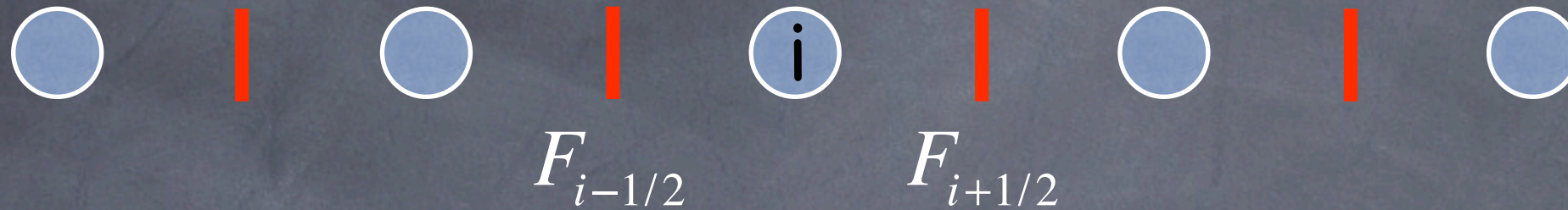
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Low-order flux that guarantees, say, monotonicity.

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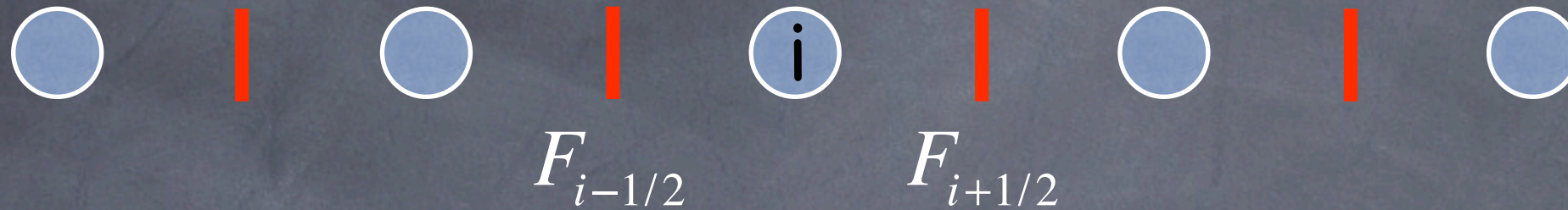
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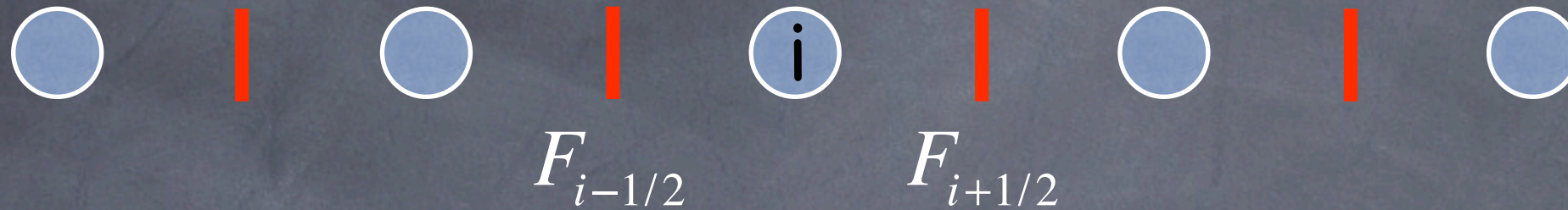
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The name of the game is to maximize ϕ while still maintaining some constraint on the tracer field (e.g. monotonicity). This can be an iterative procedure (i.e. guess ϕ , find new q , guess new ϕ ,) or it can be a deterministic where a suboptimal value of ϕ results.

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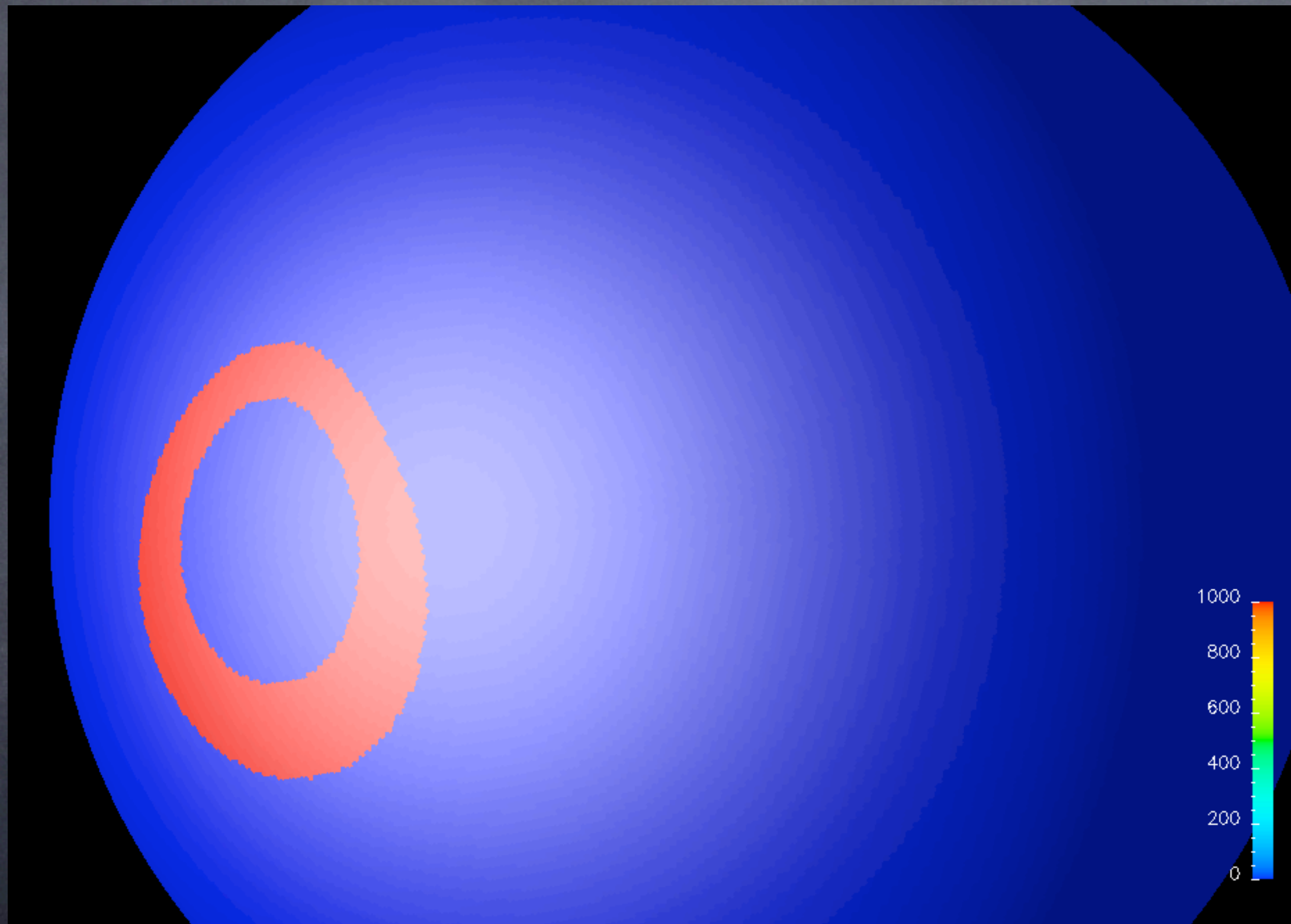
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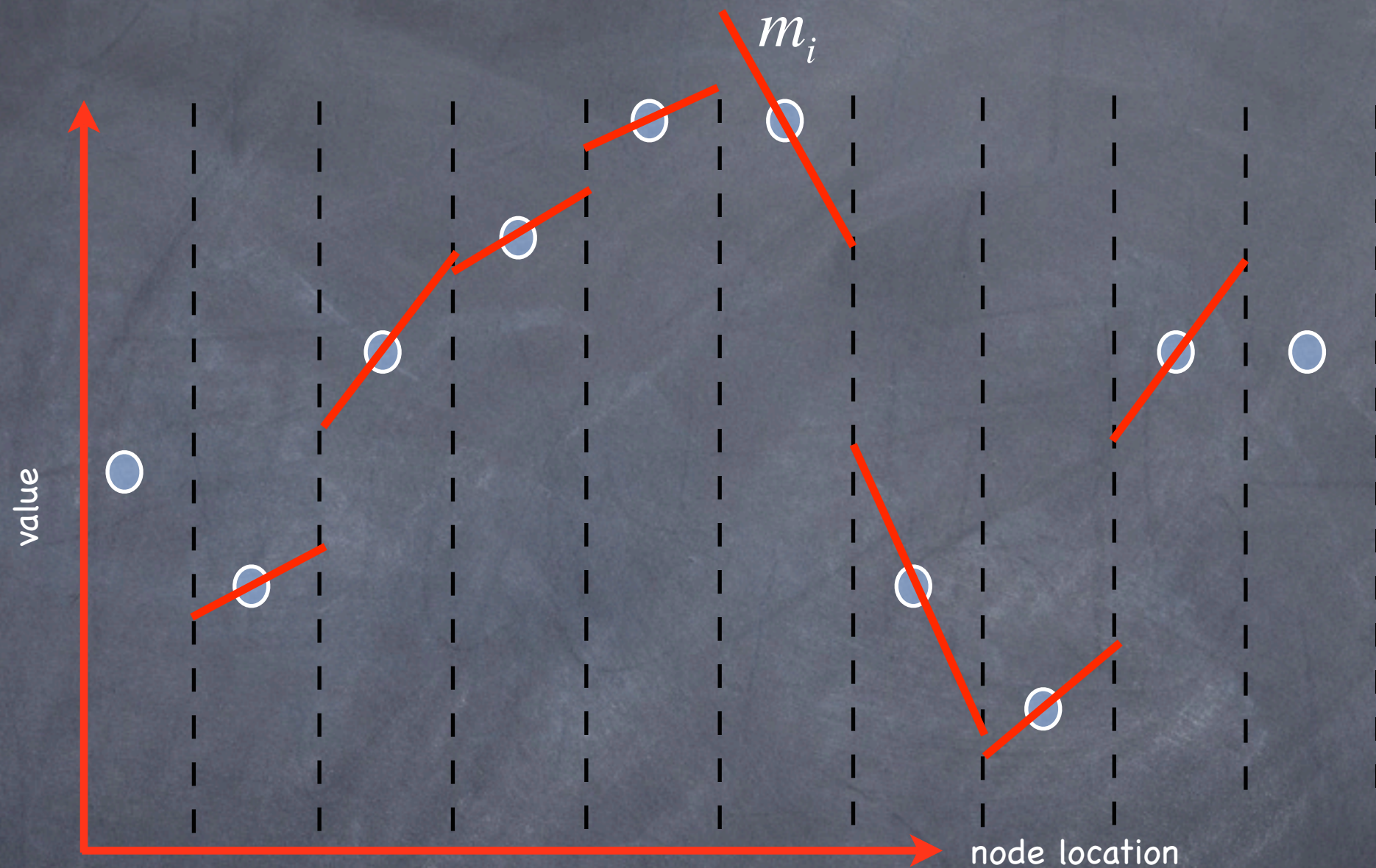
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$$\text{Note: } \hat{q}_{i+1/2}^{final} = F_{i+1/2} / M_{i+1/2} \quad \min(\hat{q}_{i+1/2}^{LOW}, \hat{q}_{i+1/2}^{HIGH}) \leq \hat{q}_{i+1/2}^{final} \leq \max(\hat{q}_{i+1/2}^{LOW}, \hat{q}_{i+1/2}^{HIGH})$$

Limiting the Flux:
Limiting to maintain q as positive definite.



Approach #2: Limiting the Reconstruction



$$q_i(x) = q_{mean} + m_i(x - \bar{x})$$

$$m_i = (q_{i+1} - q_{i-1}) / (x_{i+1} - x_{i-1})$$

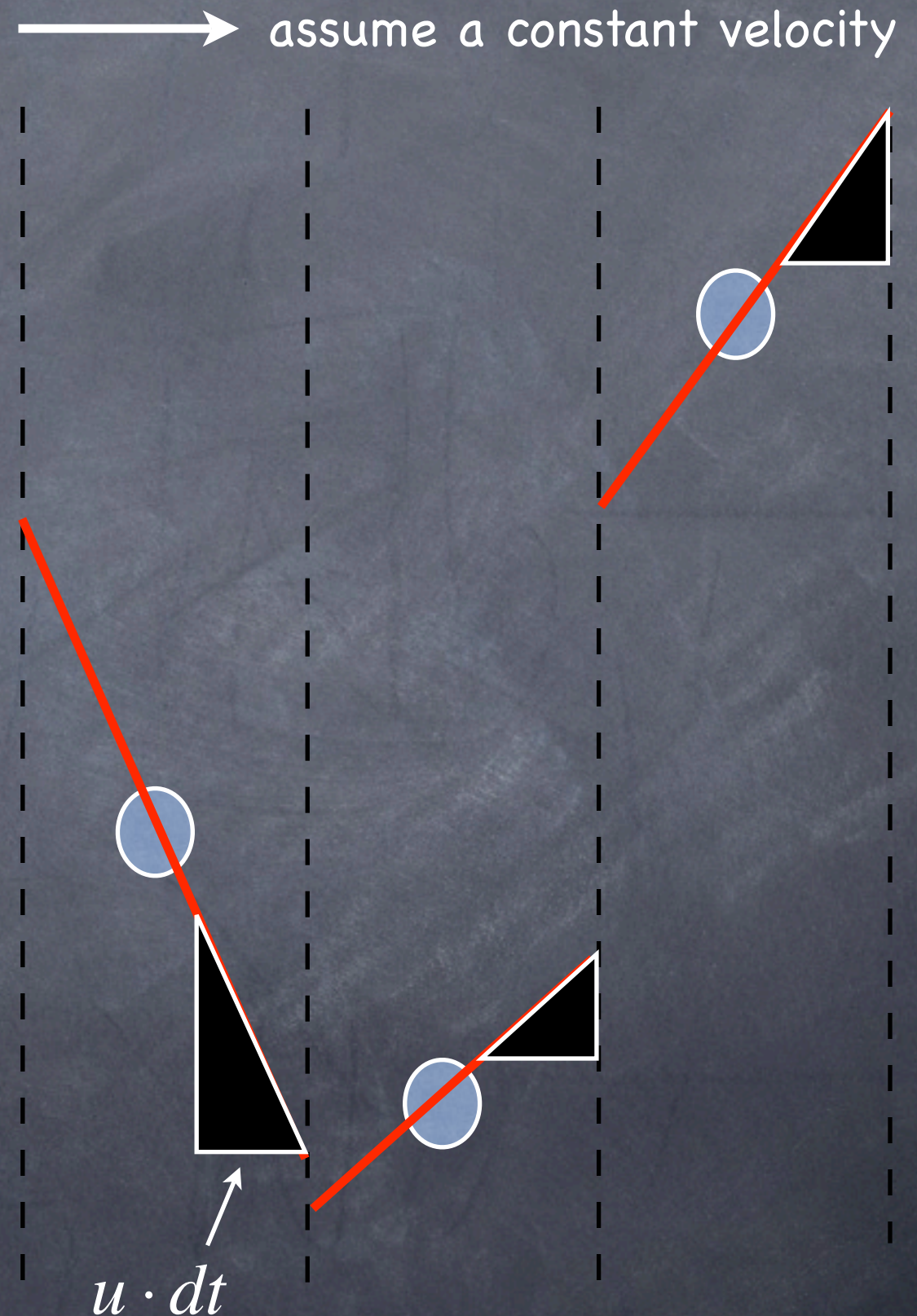
Using the reconstruction w/o modification

The flux is the "area under the curve."

$$F_{i+1/2} = \int_{\hat{x}}^{\hat{x}-u \cdot dt} q_i(\lambda) d\lambda$$

If we use the linear reconstruction without modification, we will have a 2nd-order accurate transport scheme that will, in general, create new extrema (i.e. have significant dispersive error).

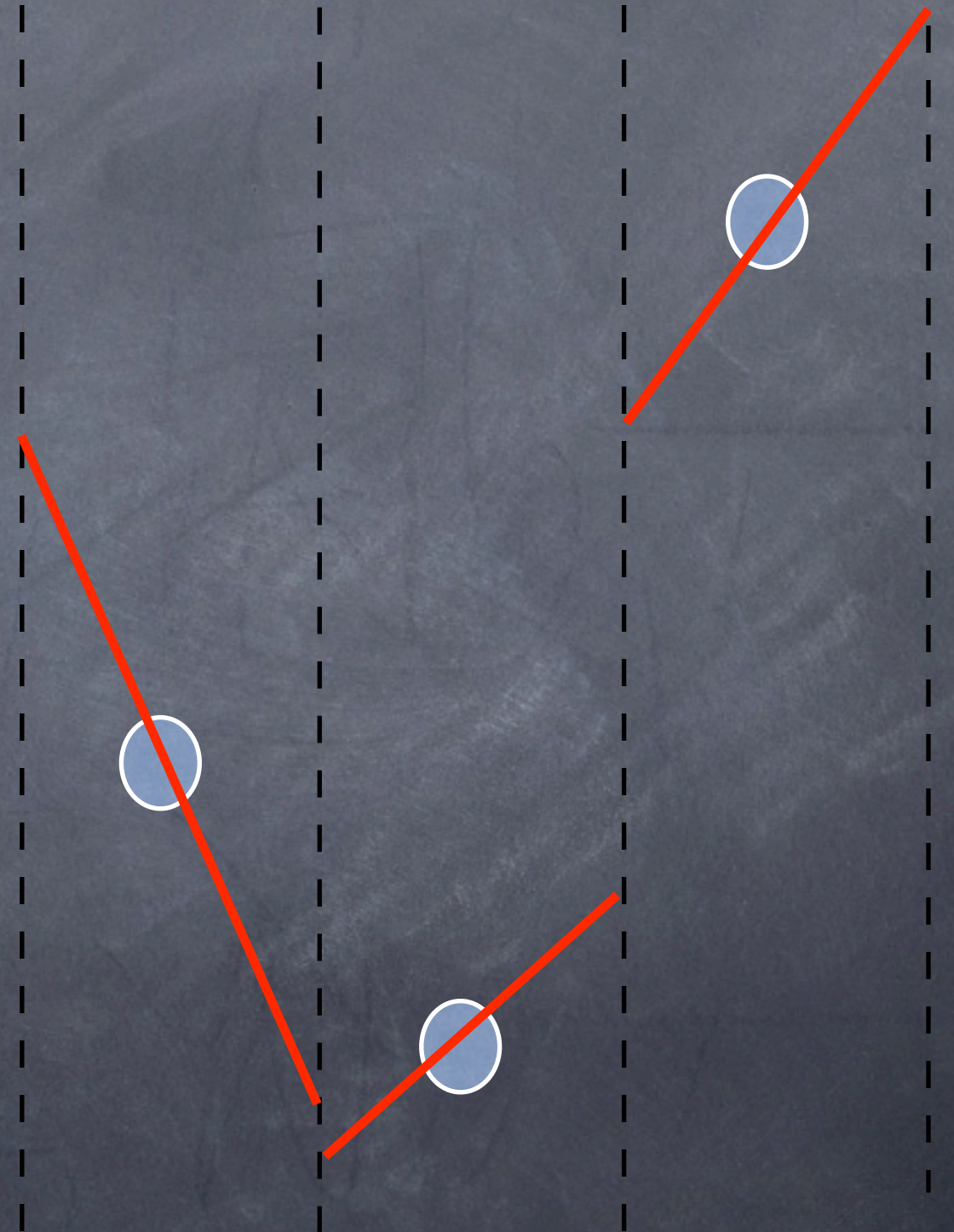
The question is how can we limit the reconstruction in order to maintain, say, a monotone transport scheme?



Using the reconstruction with limiting

First we generalize our reconstruction \longrightarrow assume a constant velocity with a limiting parameter:

$$q_i(x) = q_{mean} + \alpha_i m_i (x - \bar{x}) \quad 0 \leq \alpha_i \leq 1$$



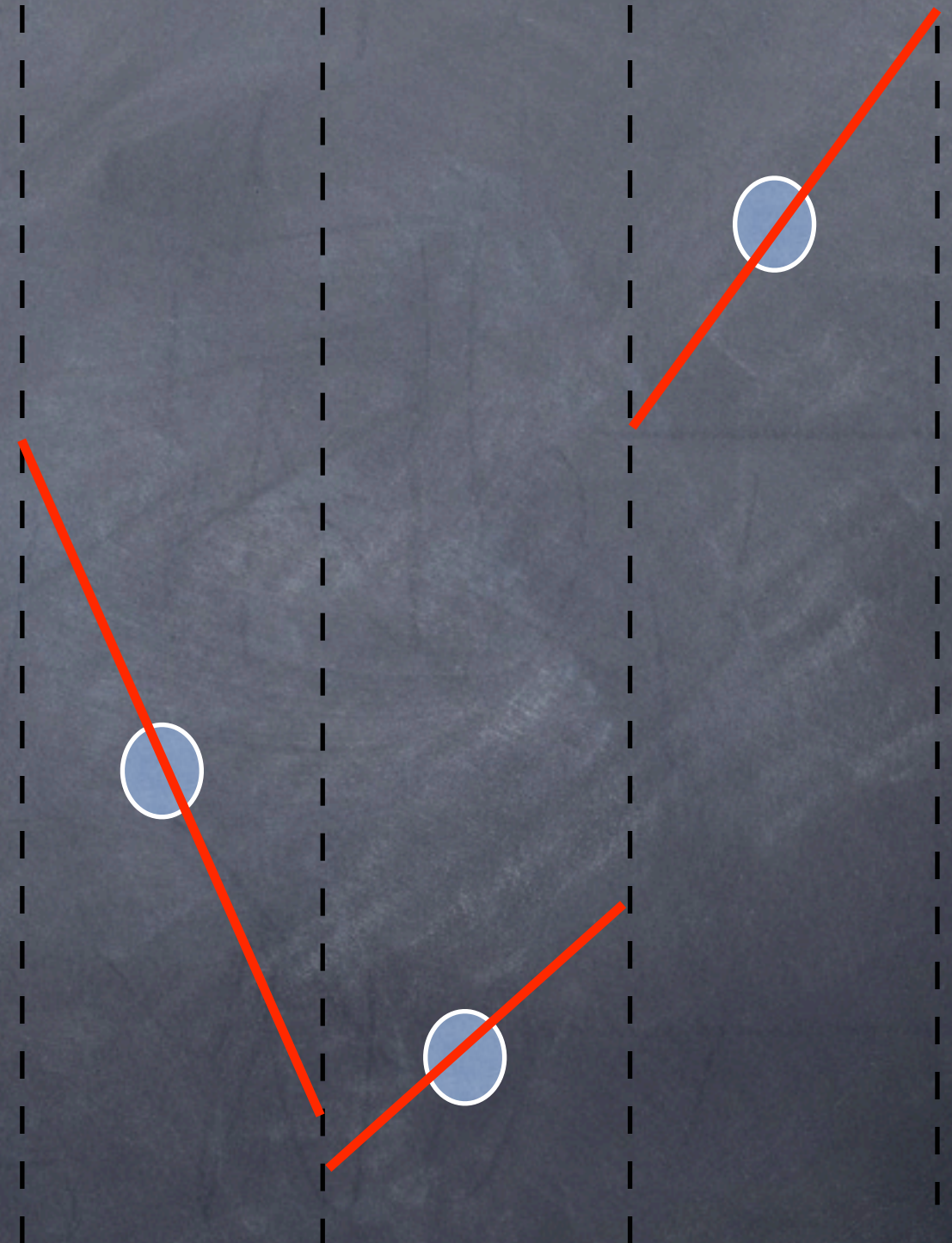
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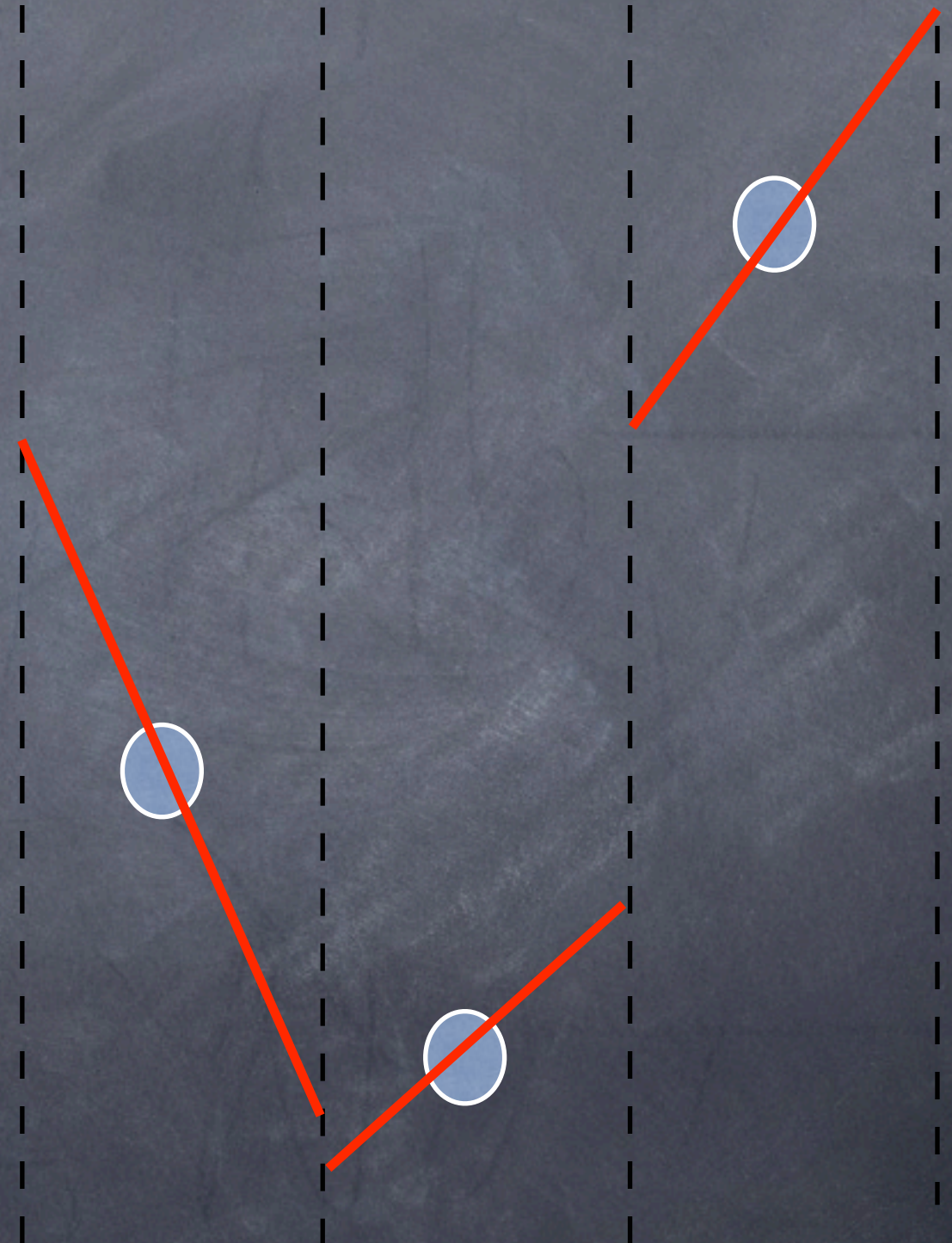
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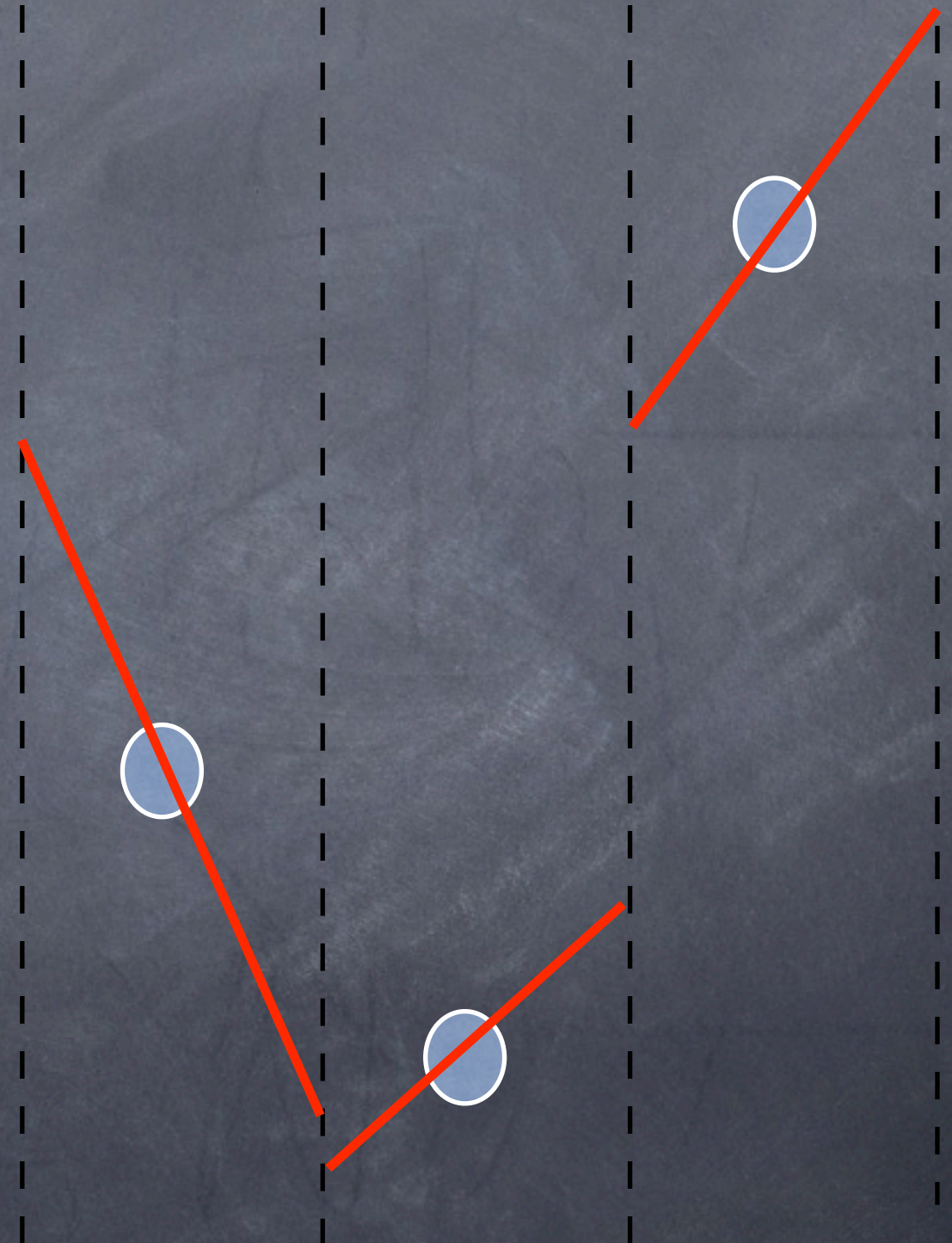
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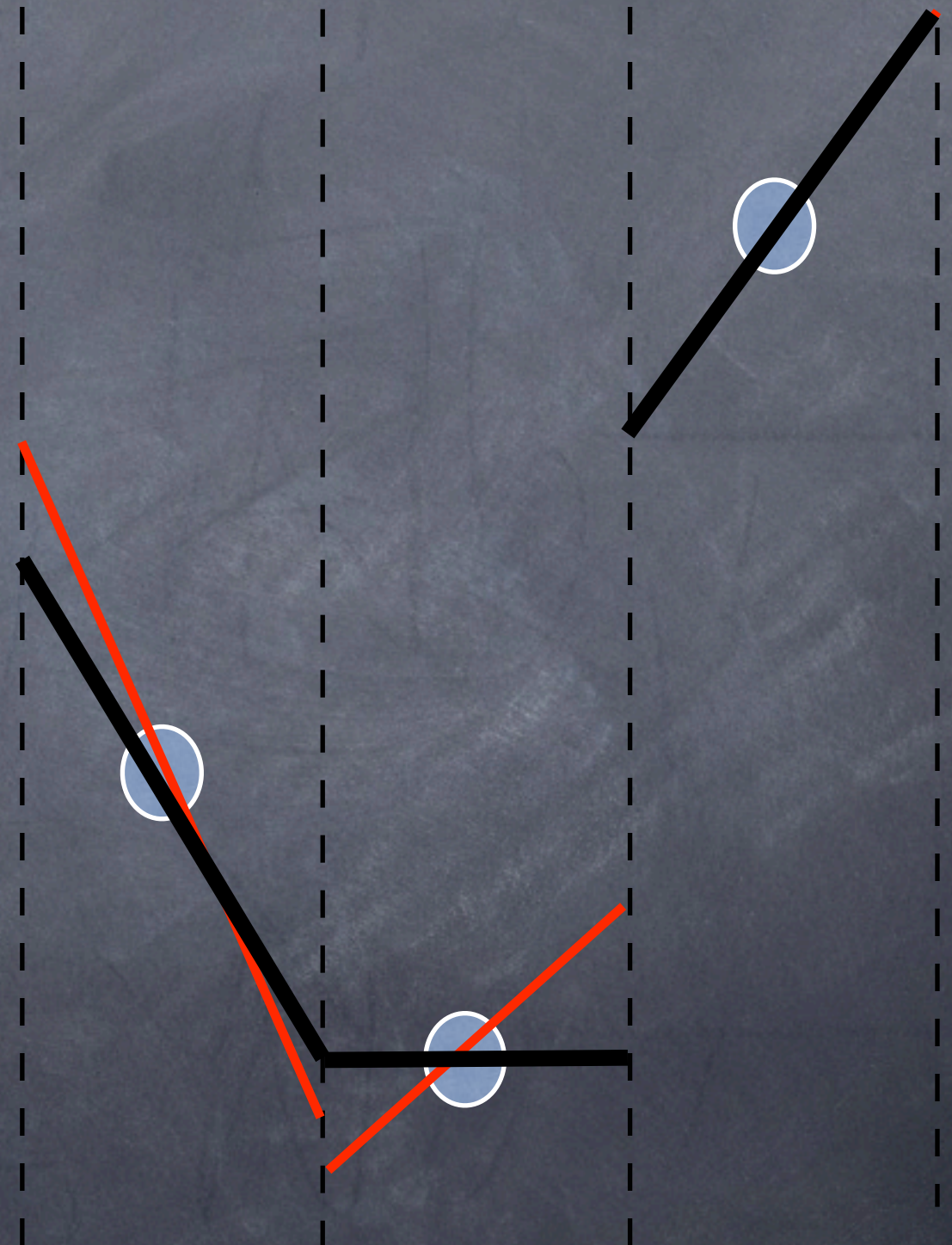
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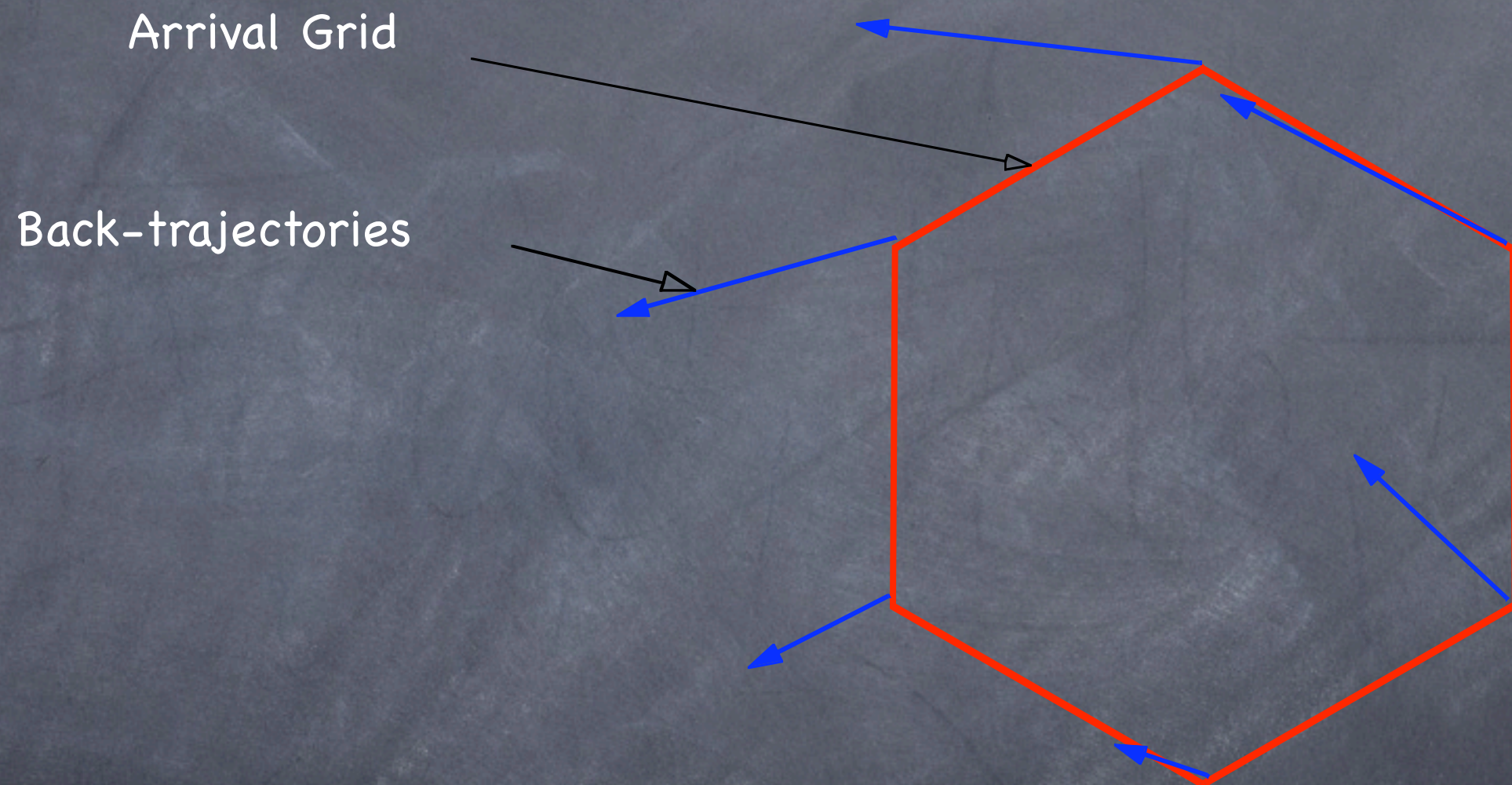
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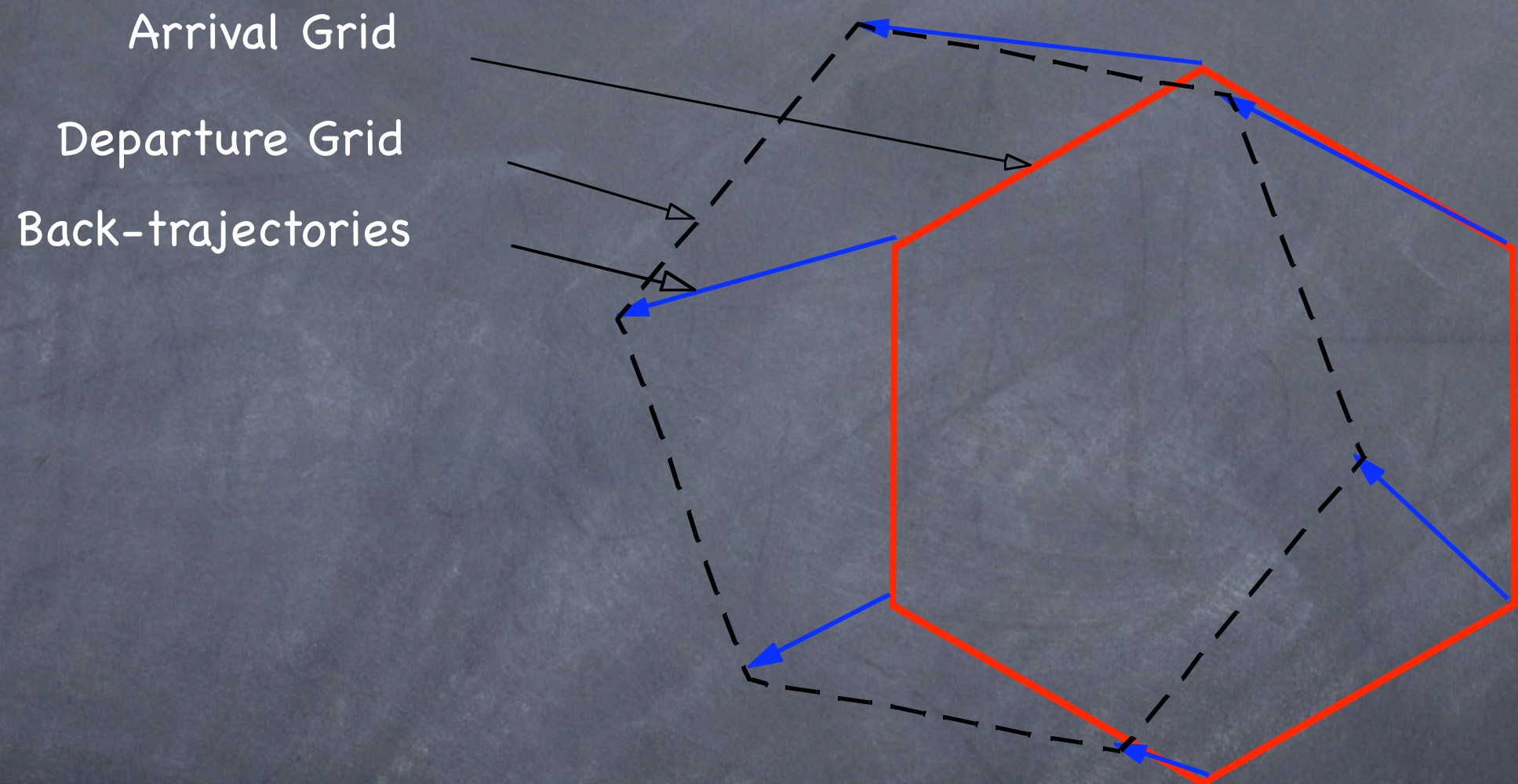
Arrival Grid



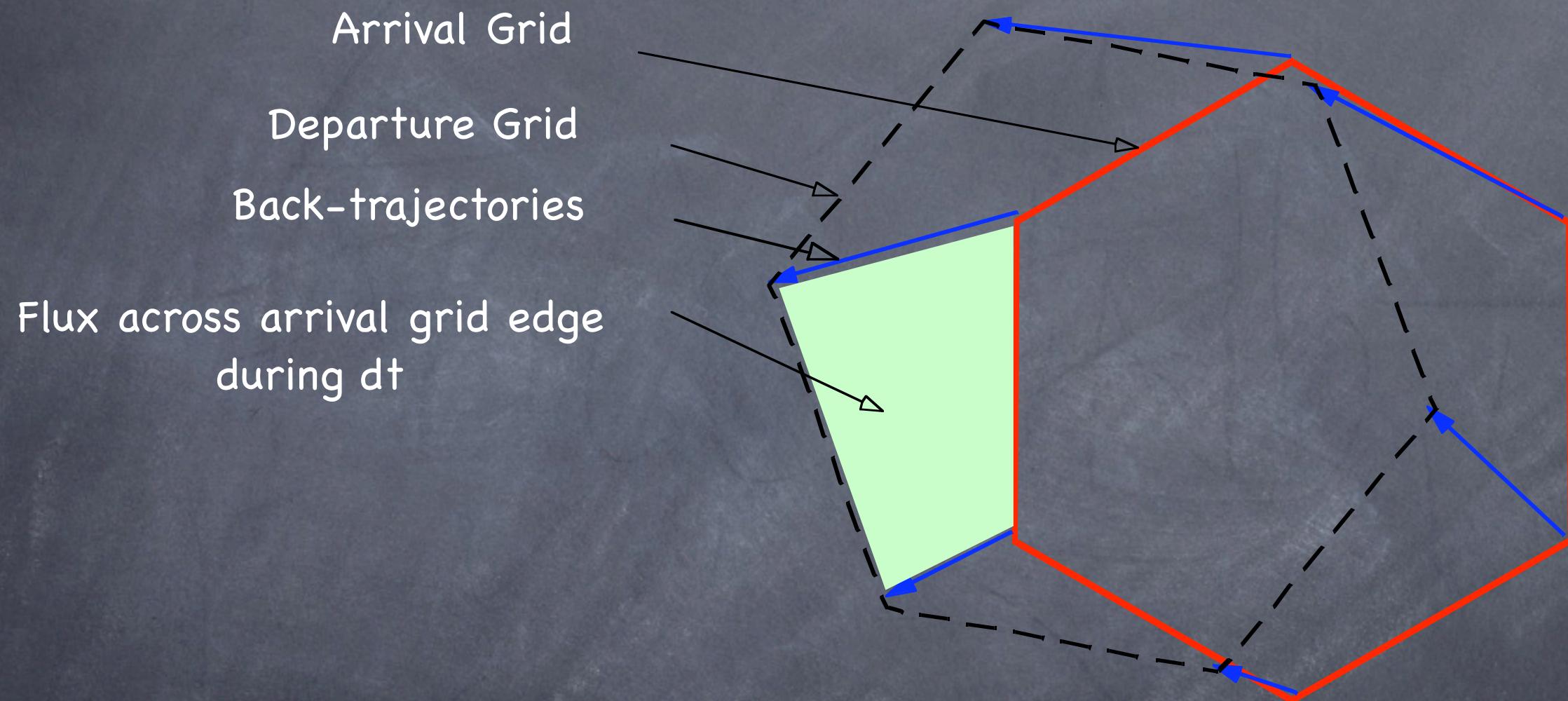
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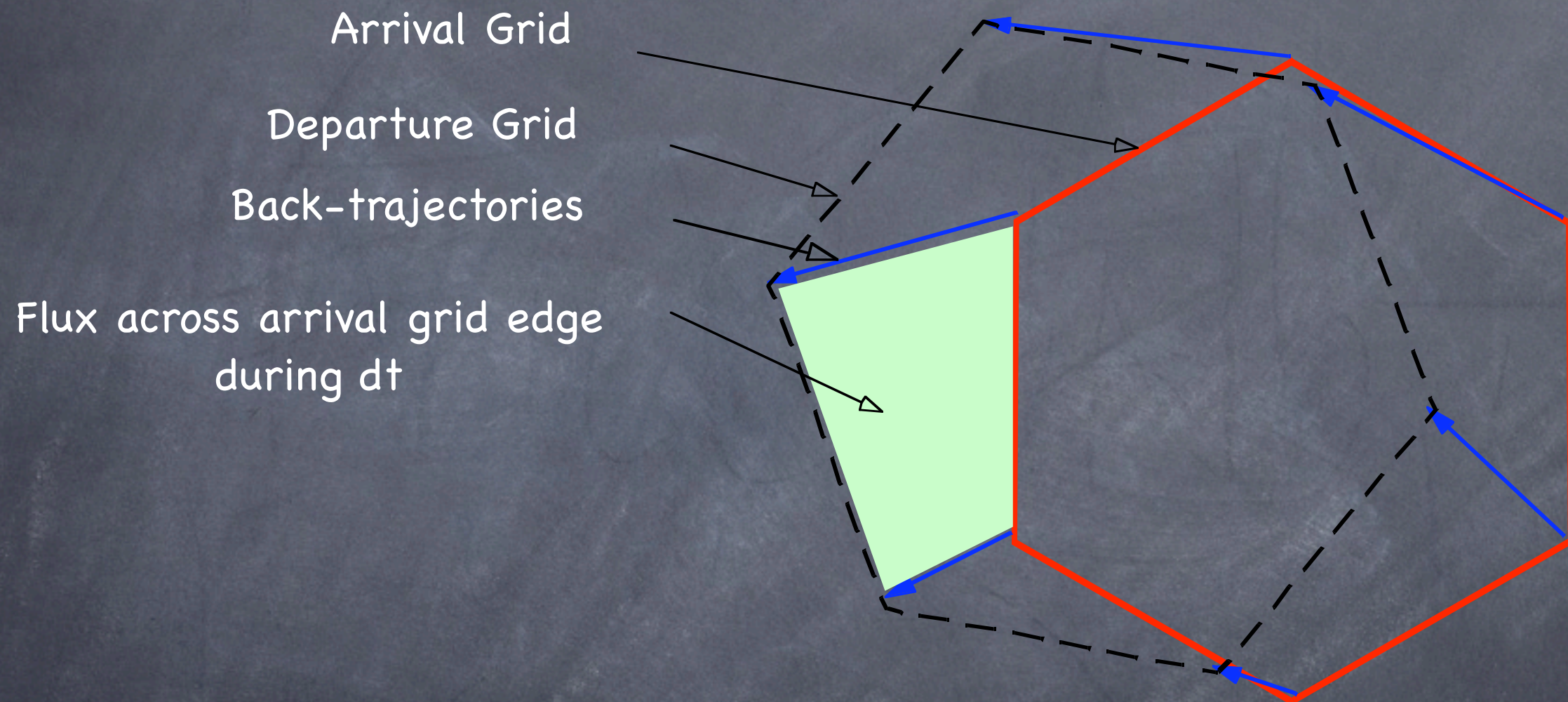
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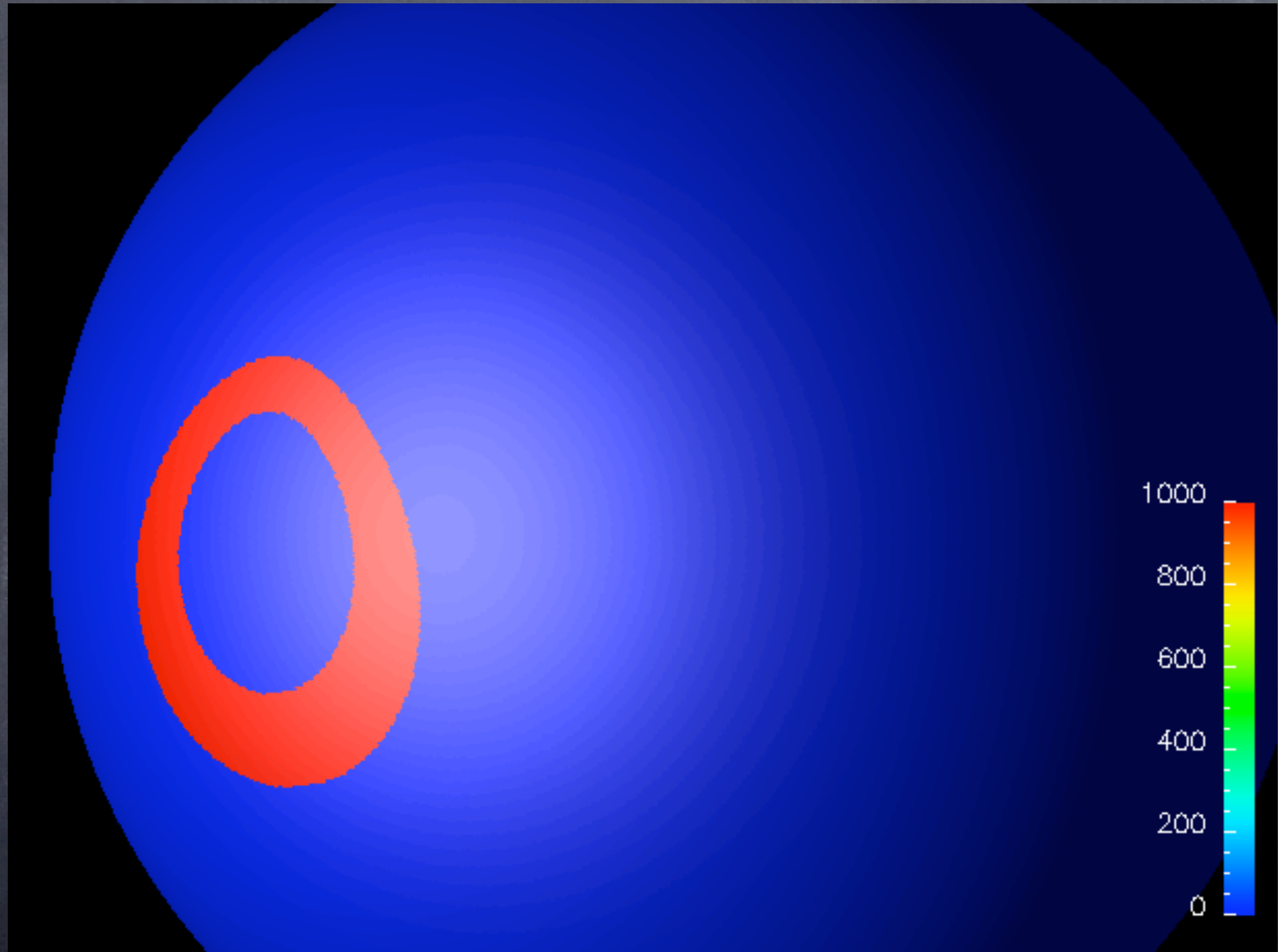


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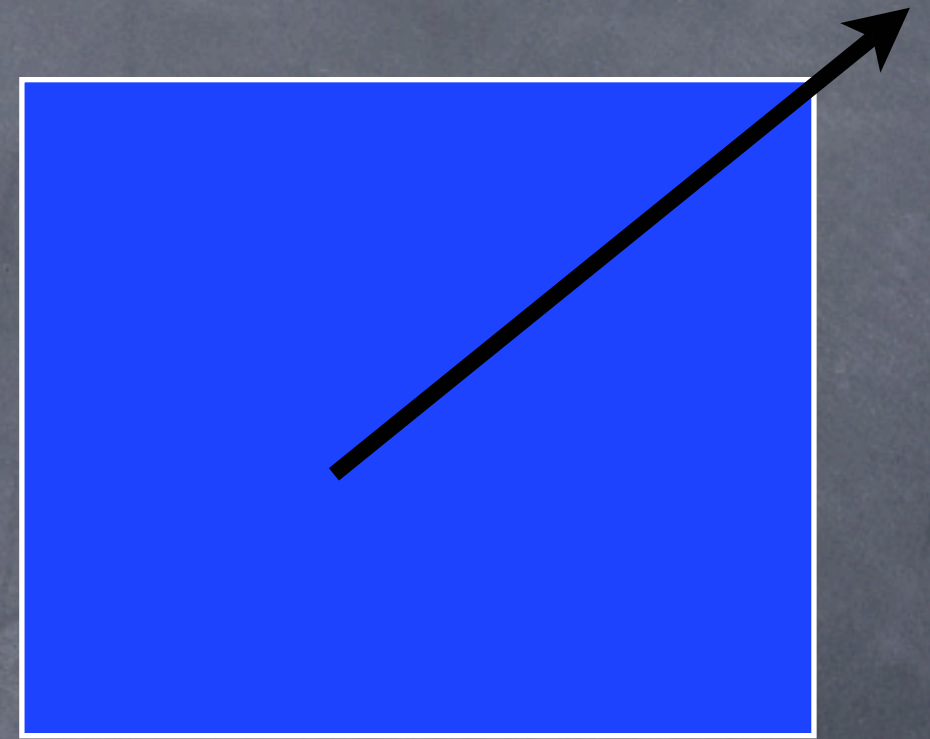


Flux is computed via quadrature methods with limiting on the reconstruction to produce a monotone (or otherwise limited) advection scheme.

Limiting the reconstruction for monotone transport

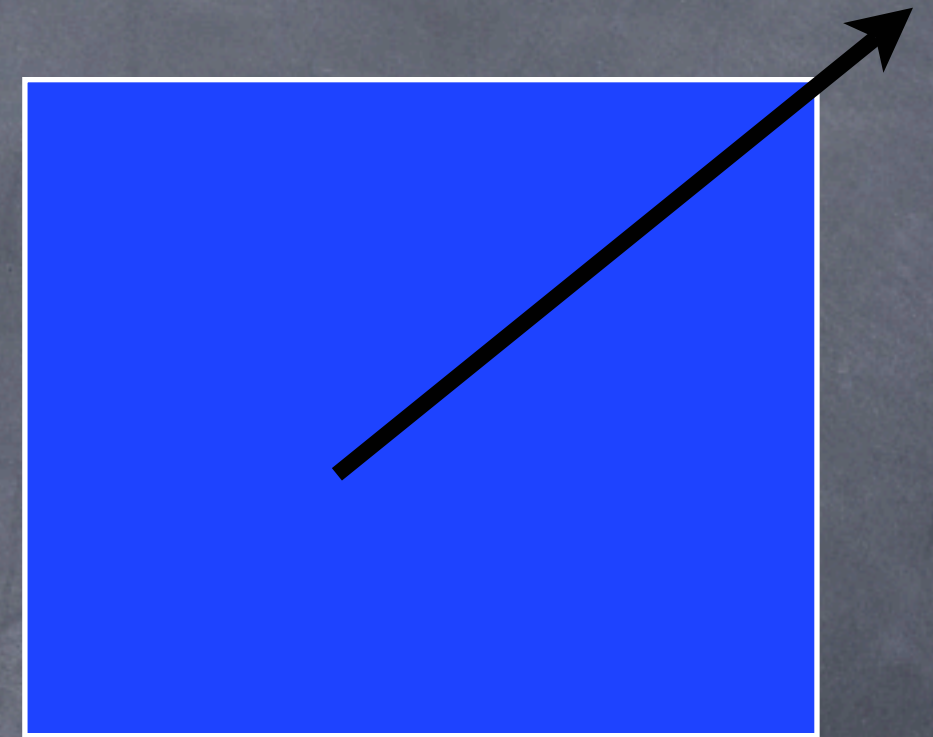


Even if we have the exact edge fluxes (and thus the exact cell mean tendency), we still have a problem



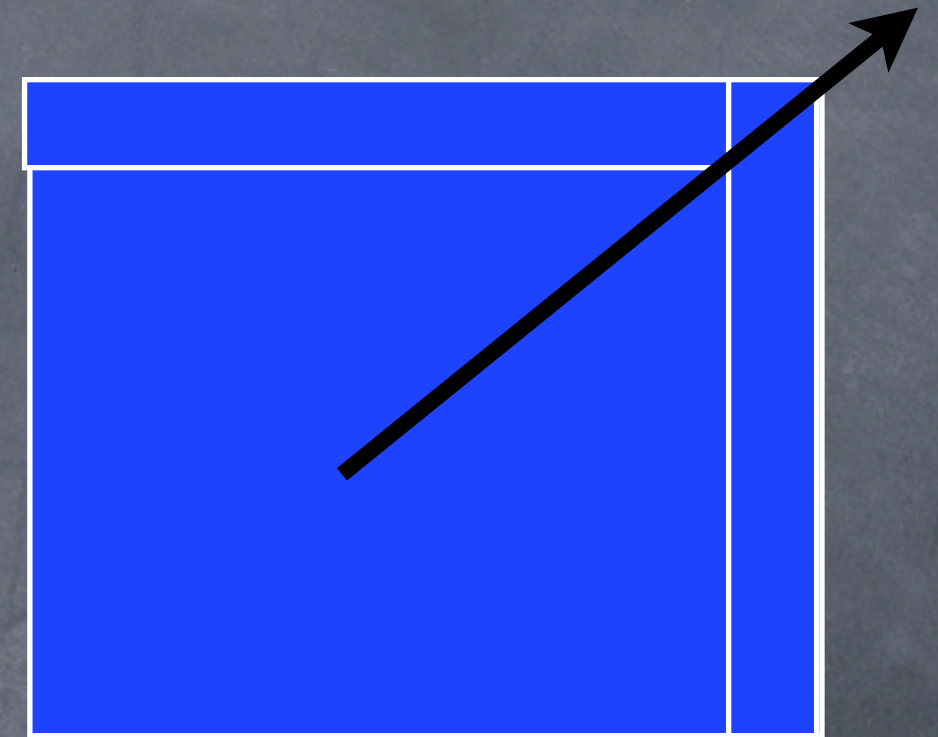
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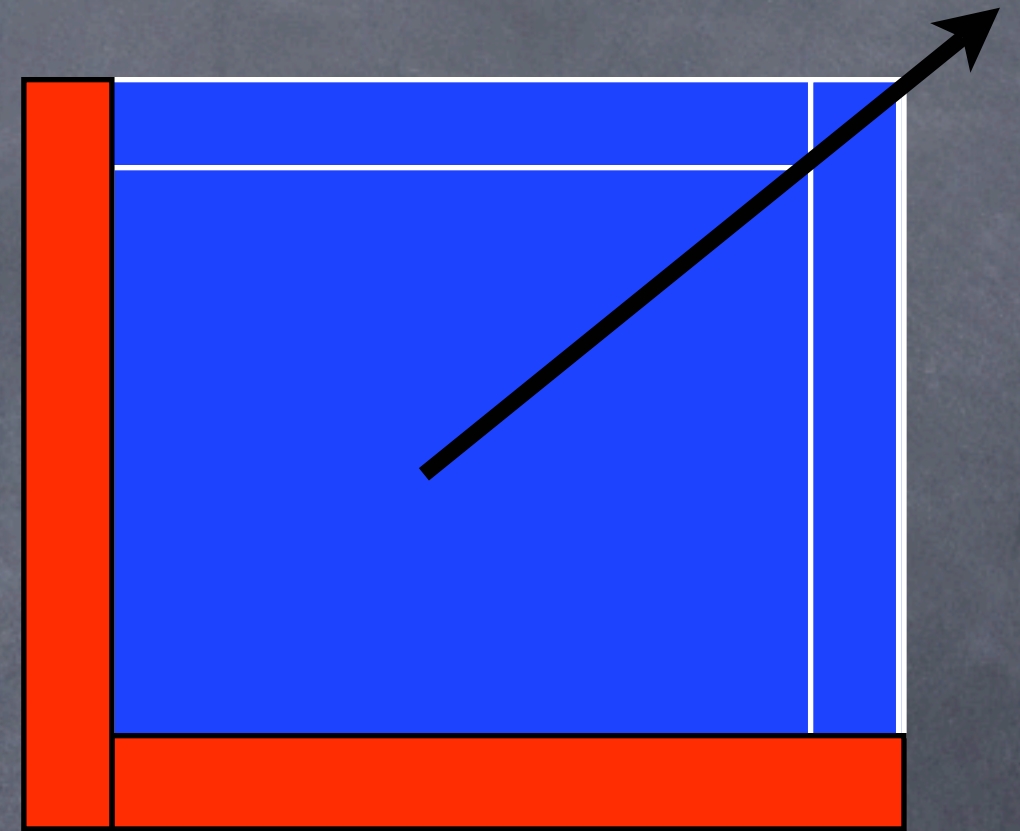
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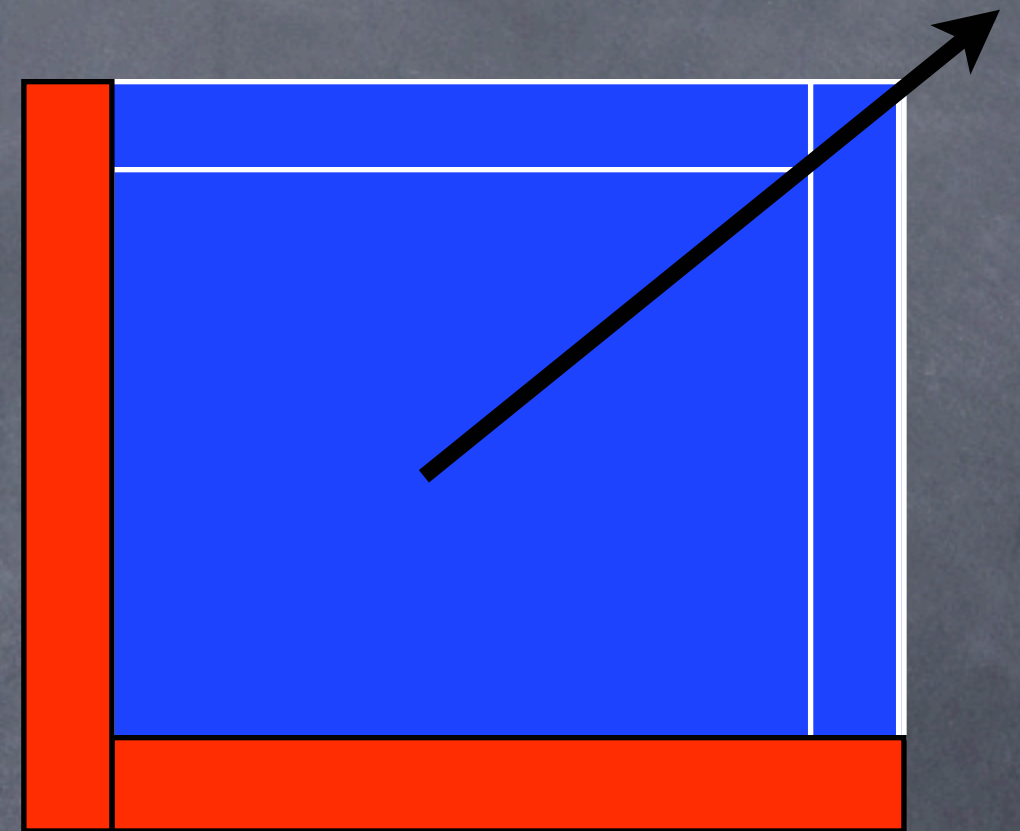
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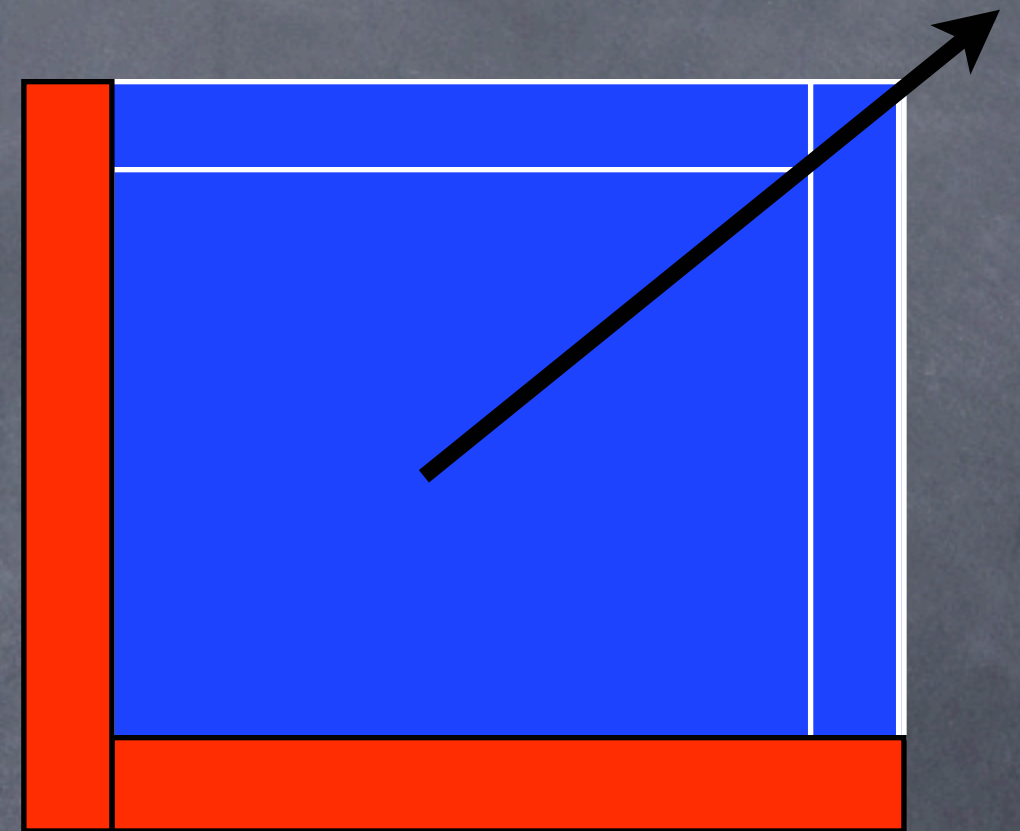
$$q^{new} = \frac{1}{A_{total}} \left[(A_{total} - A_{red}) q^{blue} + A_{red} q^{red} \right]$$



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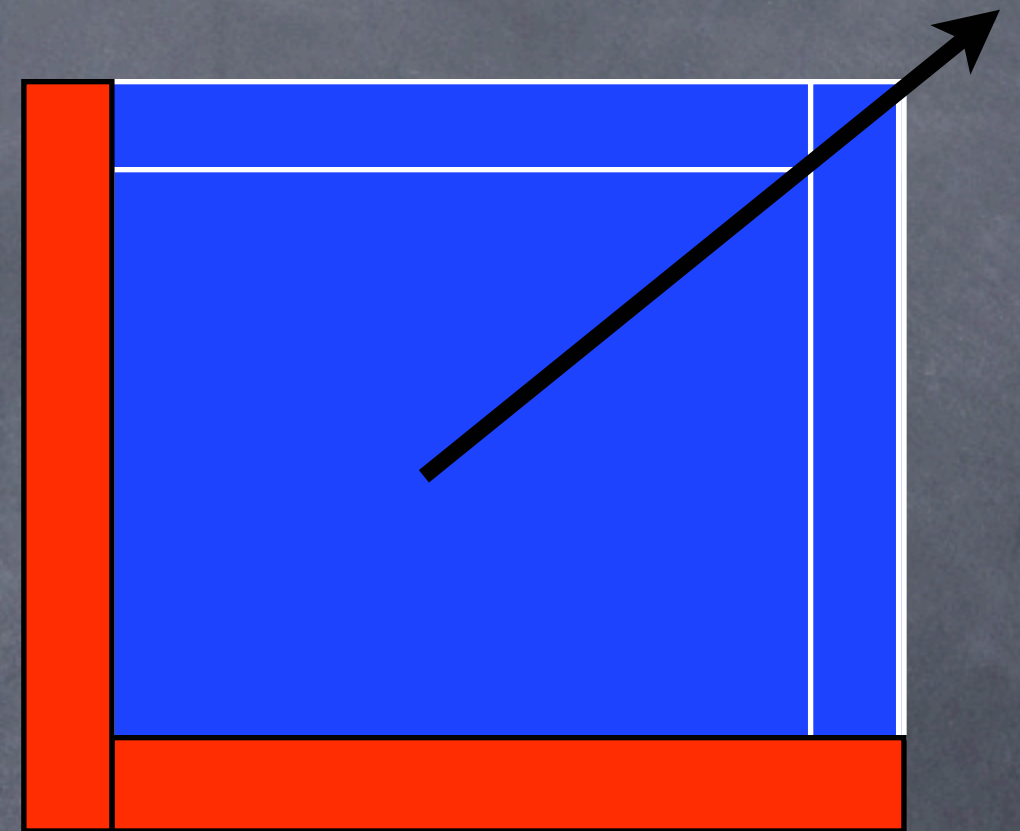


The high concentration tracer coming into the box is **immediately mixed** with the the low concentration tracer left in the box.

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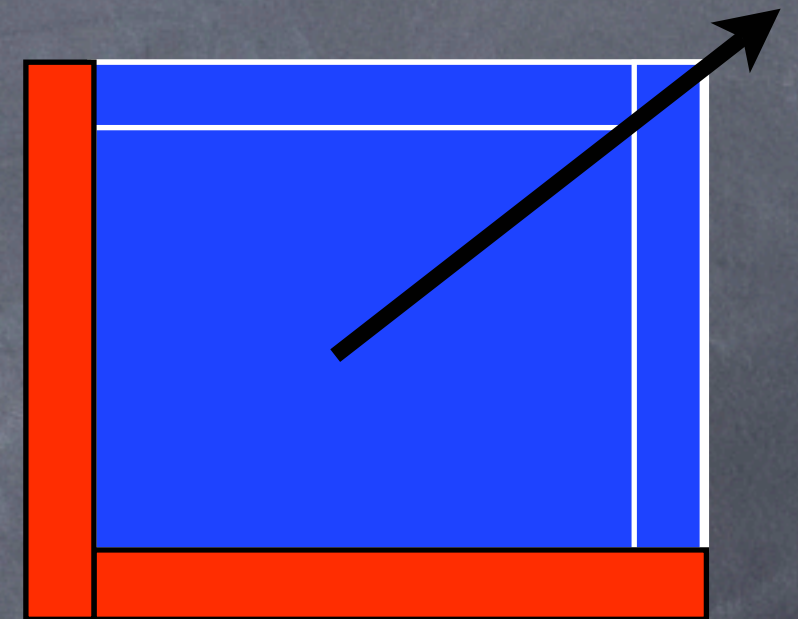
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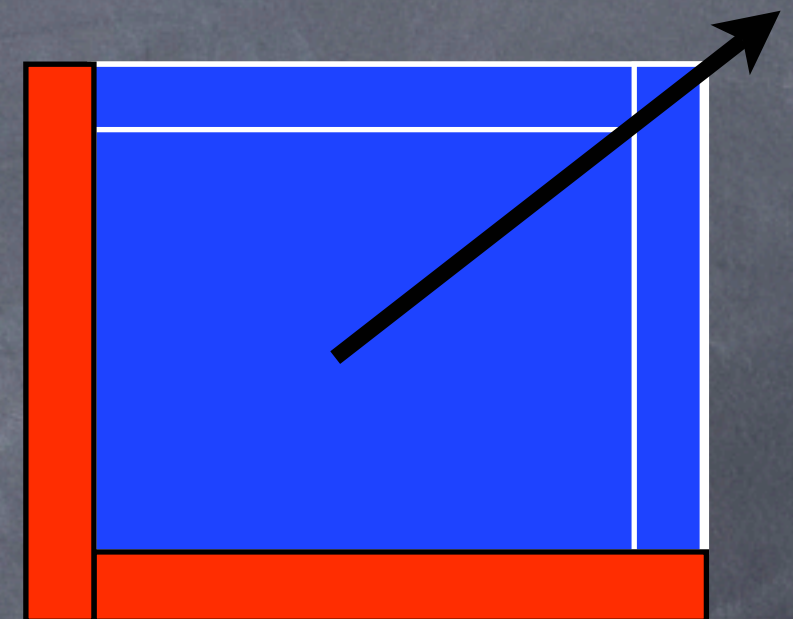
On the next time step, the (now diluted) high tracer that came in the left side of the box will exit out the right side of the box, regardless of the size of the box!

This mixing occurs because we (generally) only keep track of the cell mean quantity, so one (rather expensive) way around this problem is to augment our cell-mean tracer equation with tracer-moment equations that allow us to retain the information that “red” is to the bottom-left.



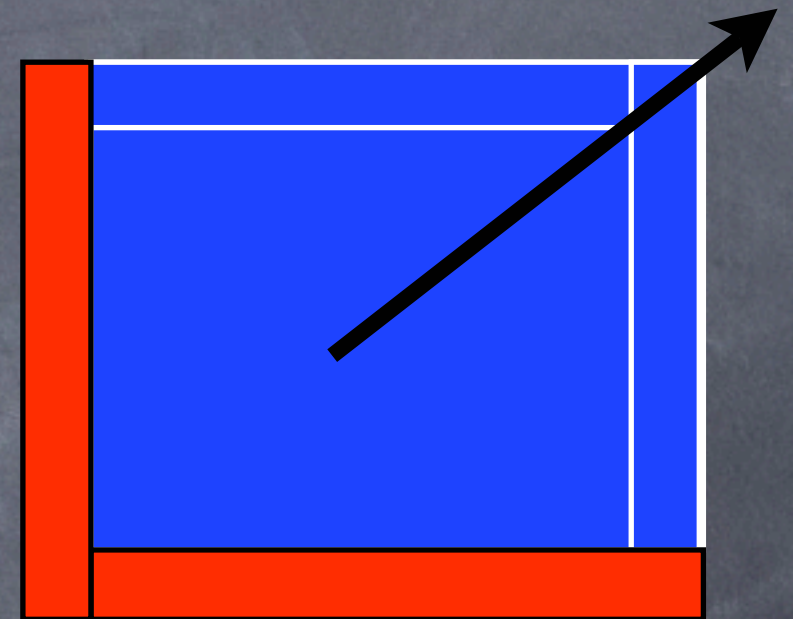
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In addition to conserving the zeroth-moment of the tracer field, we also conserve the first, or maybe even, the second moments. At this point the distinction between finite-volume and discontinuous Galerkin becomes unclear.



This mixing occurs because we (generally) only keep track of the cell mean quantity, so one (rather expensive) way around this problem is to augment our cell-mean tracer equation with tracer-moment equations that allow us to retain the information that “red” is to the bottom-left.

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$$q(x, y) = m_0 K_0 + m_x K_x + m_y K_y + \dots$$

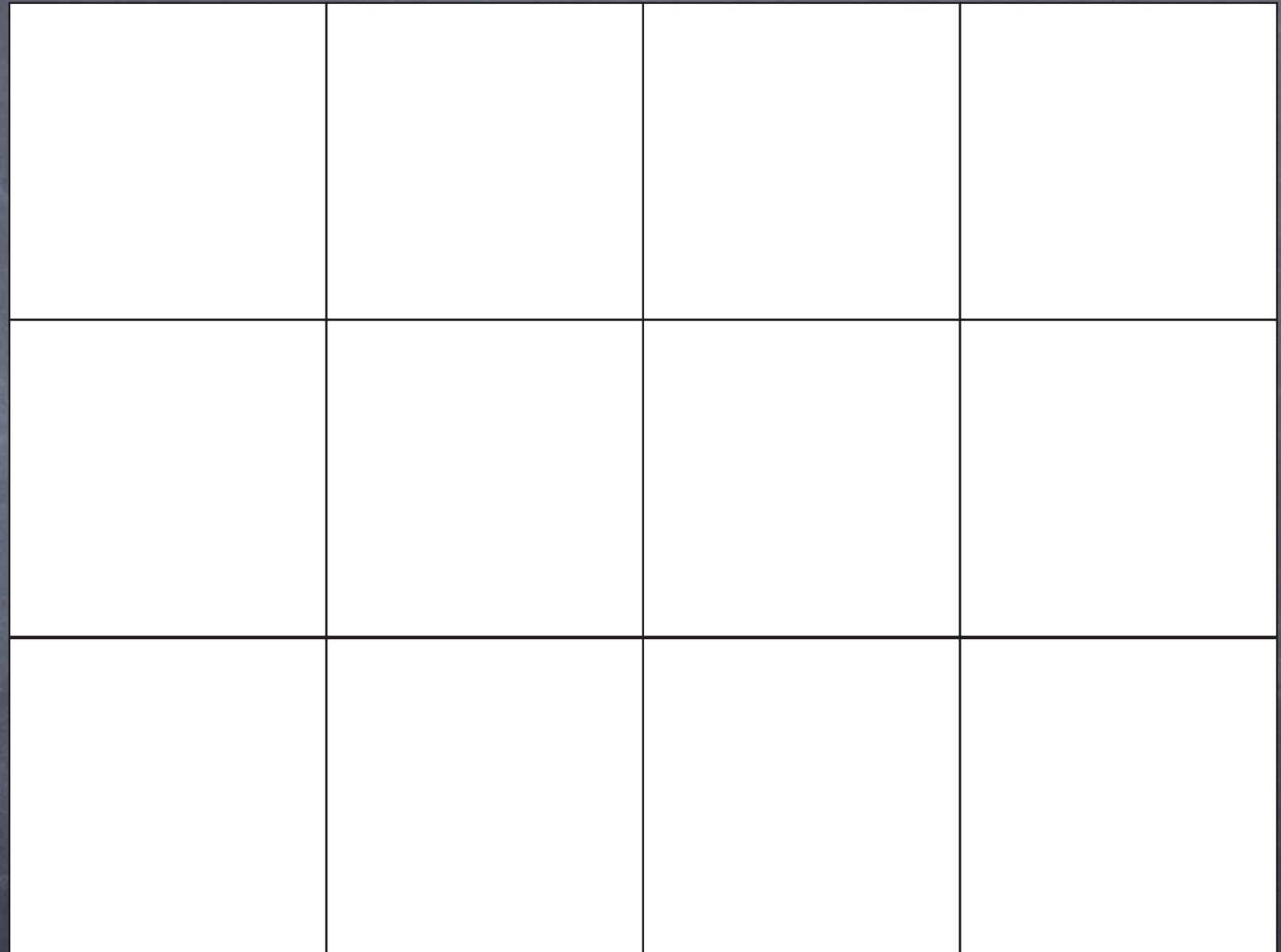
$$K_0 = 1, K_x = x - \bar{x}, K_y = y - \bar{y} \quad \leftarrow \text{our orthogonal basis}$$

evolution equations for m_0, m_x, m_y, \dots


cell-mean value $\xrightarrow{\quad\quad\quad}$ $\xrightarrow{\quad\quad\quad}$ $\xrightarrow{\quad\quad\quad}$ tracer slope in x,y directions

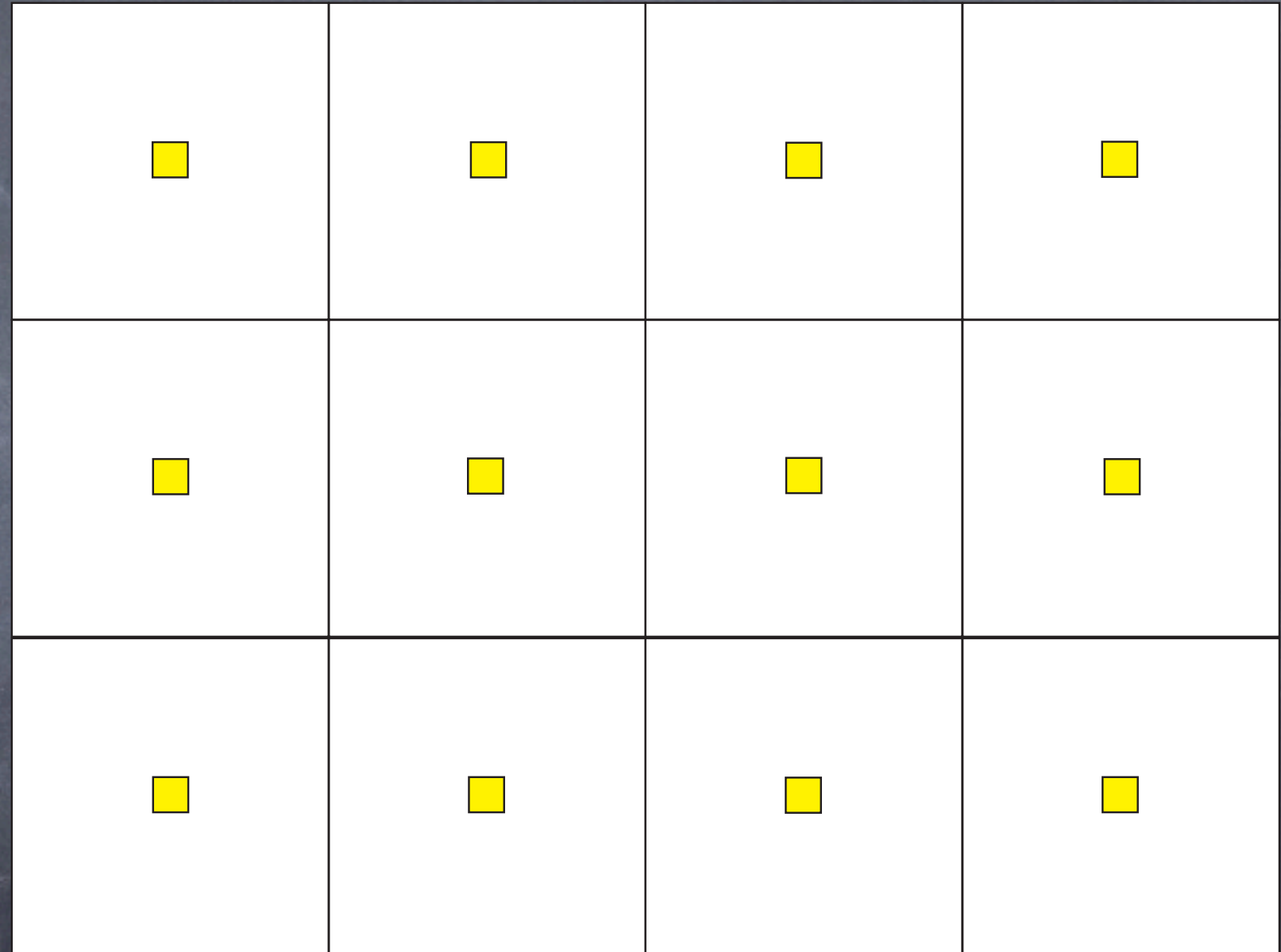
And finally, a tie back to Monday's discussion on $F=ma$ and "slaving" the velocity field to our discrete vorticity equation.

RECAP: What is the C-grid staggering?

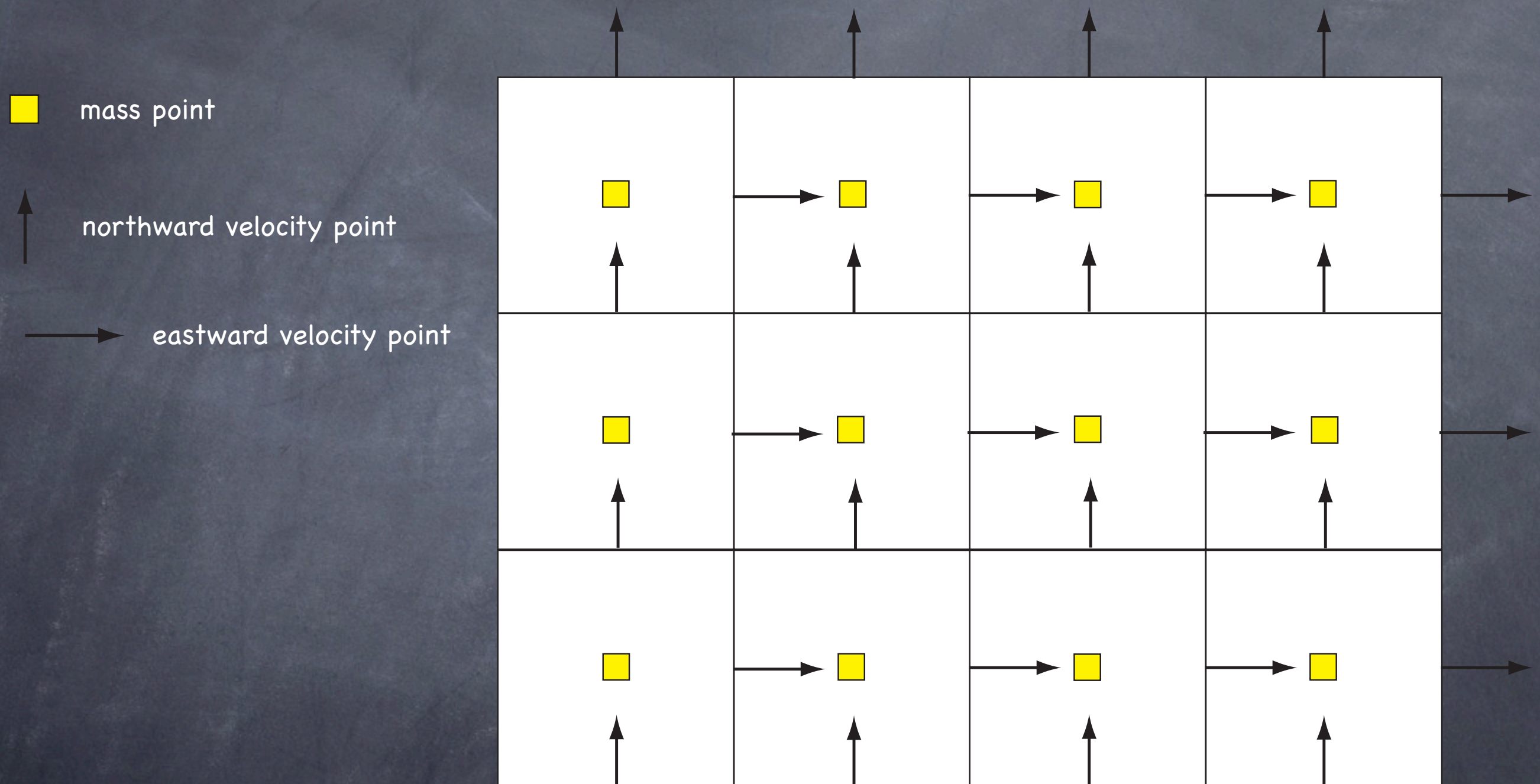


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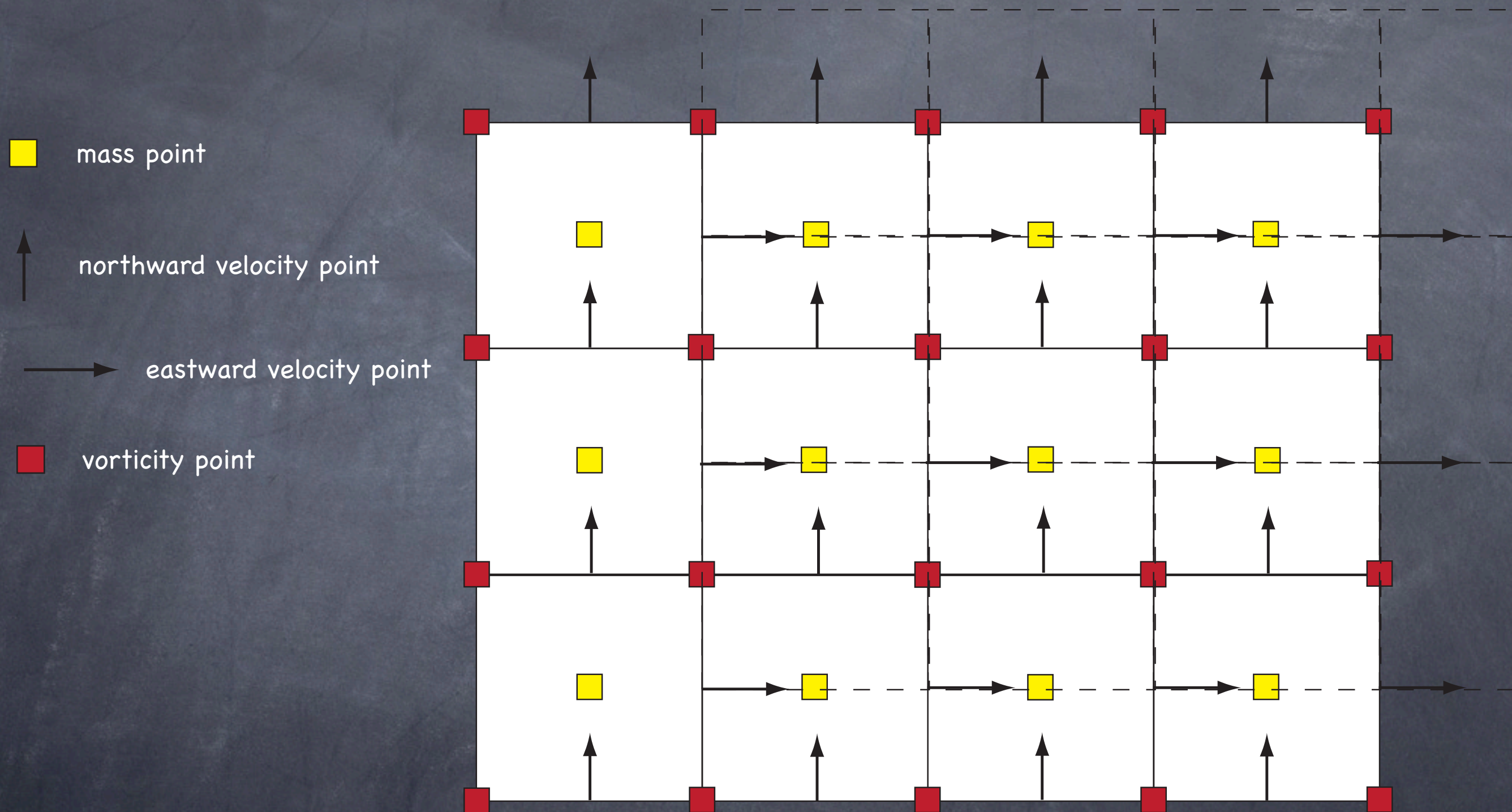
 mass point



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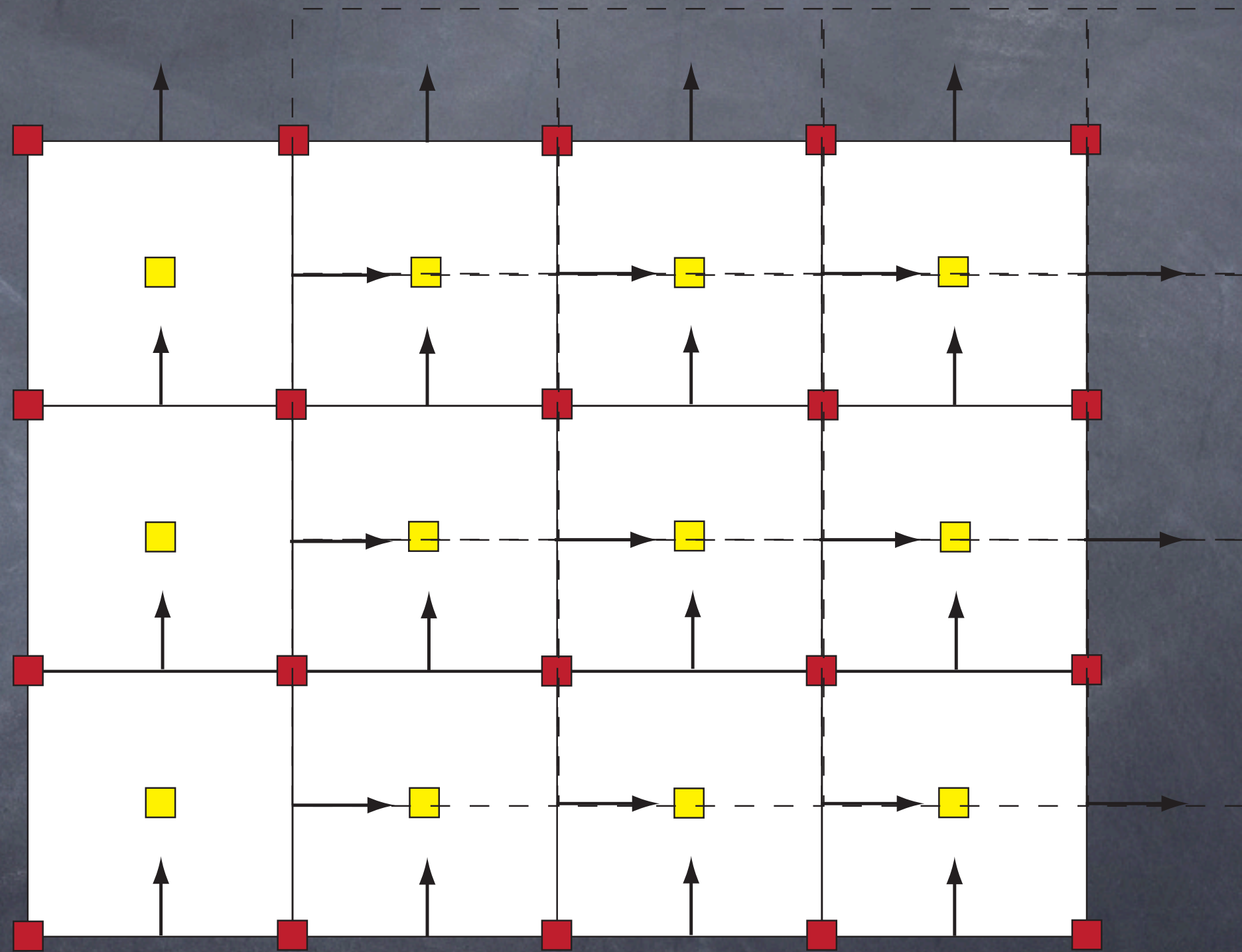
■ mass point

↑ northward velocity point

→ eastward velocity point

■ vorticity point

Define all prognostic velocity points as N (as in Normal) to a mass cell edge. In order to construct a full velocity vector, N will have be augmented with T (as in Tangent) to a mass cell edge, defined positive in the $\mathbf{k} \times \mathbf{N}$ direction.



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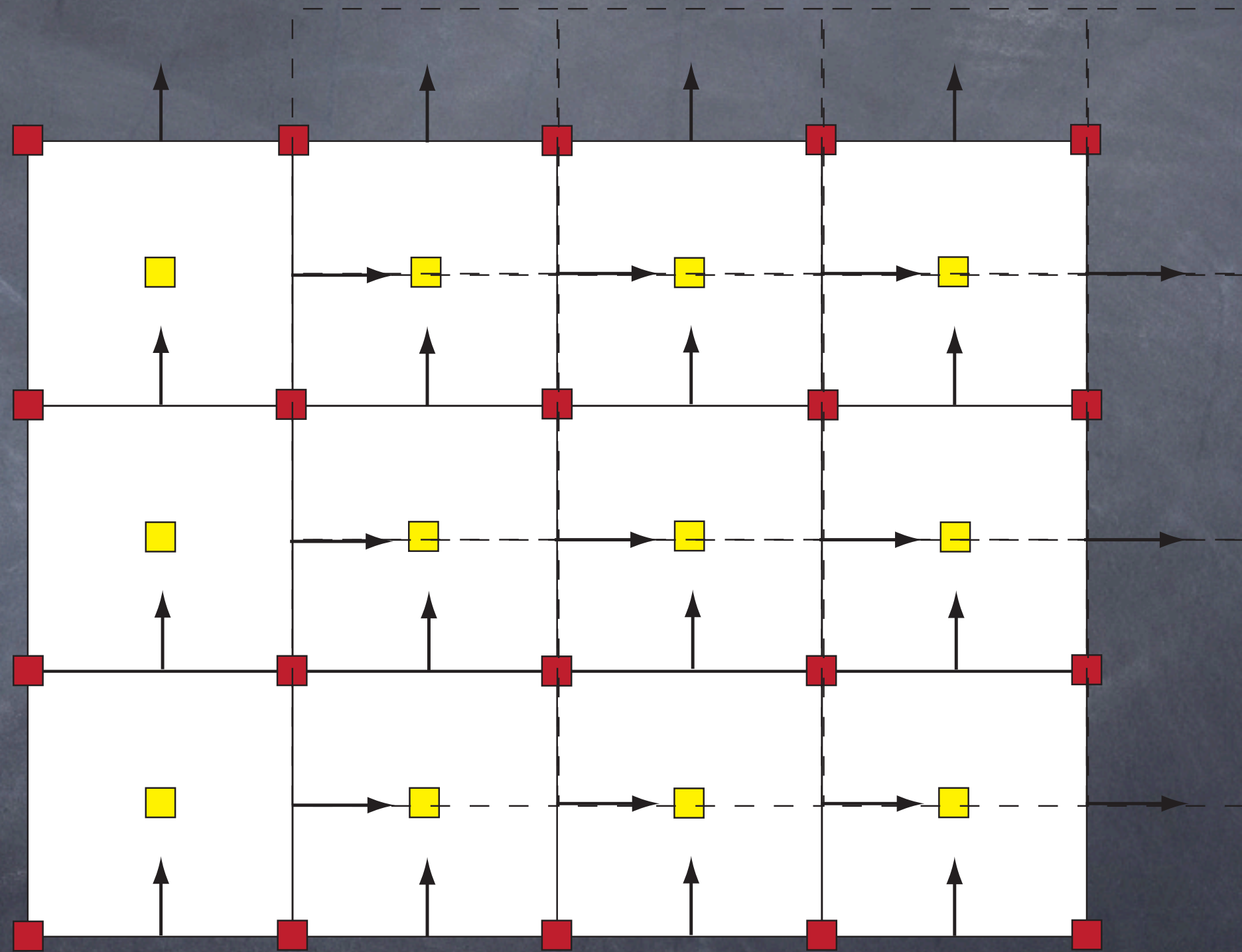
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The orthogonality constraint requires the line connecting two mass points to be orthogonal to the shared edge (and thus parallel to the projected velocity component).

RECAP: The discrete momentum equation: everything with an overhat has to be defined

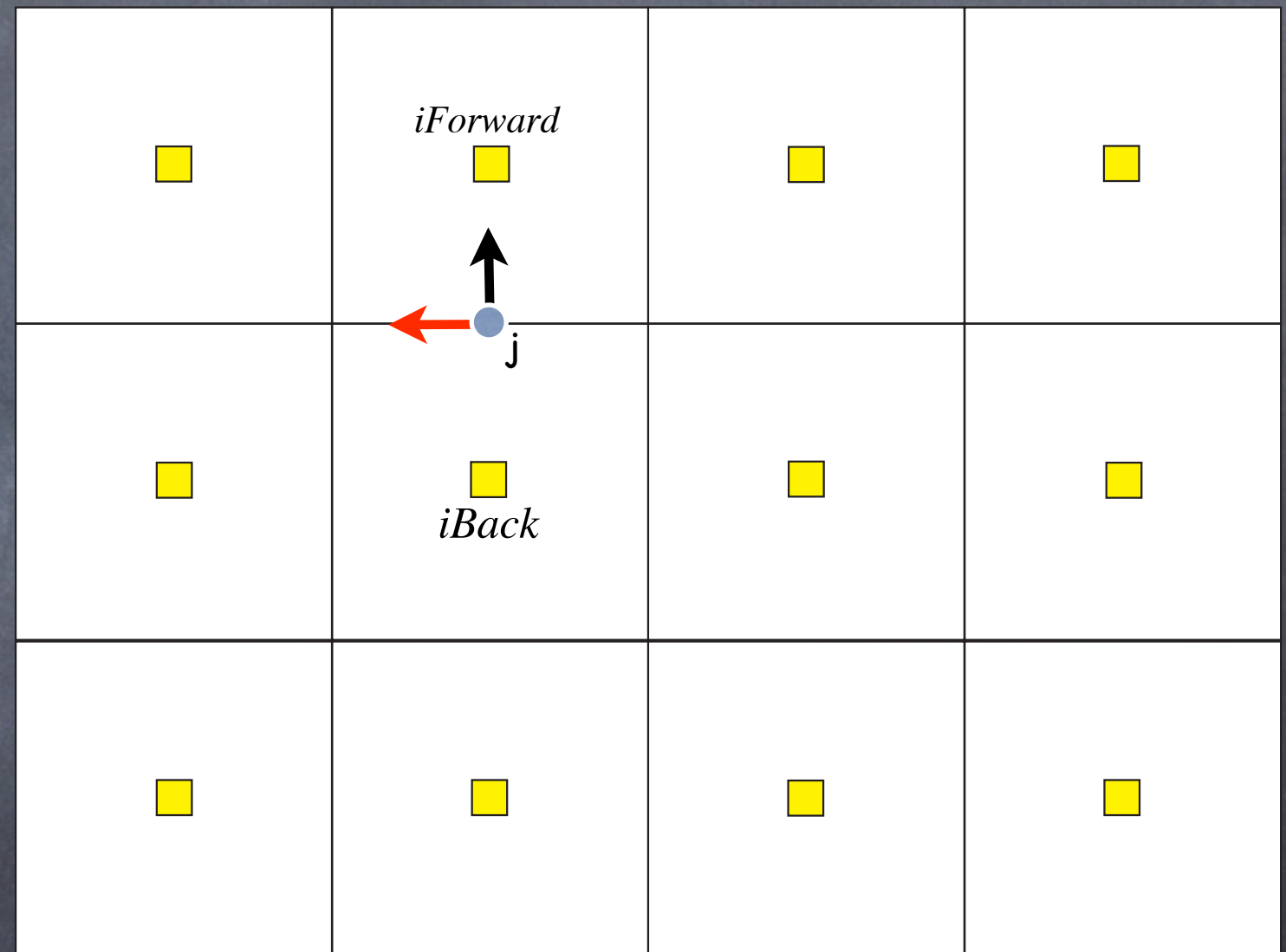
$$\frac{\partial N_j}{\partial t} = \hat{\eta}_j \hat{T}_j - \left\{ \left[gh + gh_s + \hat{K} \right]_{iForward} - \left[gh + gh_s + \hat{K} \right]_{iBack} \right\} / dc_j$$

○ dc_j distance between
iForward and iBack

○ $\hat{\eta}_j$ absolute vorticity

← \hat{T}_j reconstructed, tangent
velocity, for here simply
state $\hat{T}_j = f(N_j)$.

■ $gh + gh_s + \hat{K}$ sum of potential
and kinetic energy



■ mass point

The discrete vorticity equation:

taking the curl of the momentum equation.

$$\frac{1}{A_k} \sum_{j=1}^{nedges} dc_j \left\{ \frac{\partial N_j}{\partial t} = \hat{\eta}_j \hat{T}_j - \left\{ \left[gh + gh_s + \hat{K} \right]_{iForward} - \left[gh + gh_s + \hat{K} \right]_{iBack} \right\} / dc_j \right\}$$

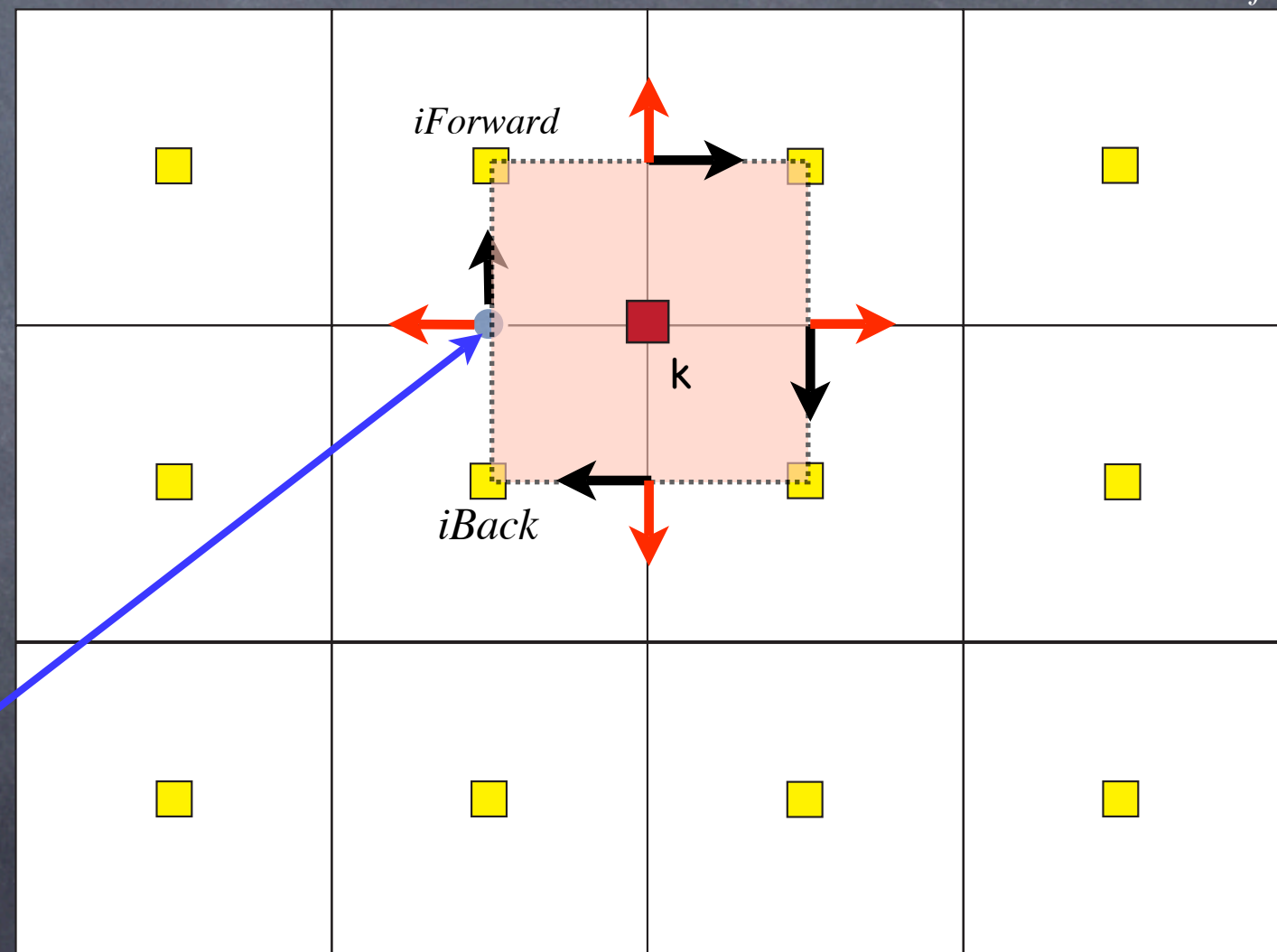
$$\frac{\partial \eta_k}{\partial t} + \frac{1}{A_k} \sum_{j=1}^{nedges} \hat{\eta}_j \hat{T}_j dc_j = 0 \quad \frac{\partial \eta}{\partial t} + \nabla \cdot (\eta \underline{u}) = 0$$

nice analog to continuous equation

$\blackrightarrow N_j$
 $\redrightarrow \hat{T}_j$

needs to be determined for use
in the momentum equation.

$\hat{\eta}_j$

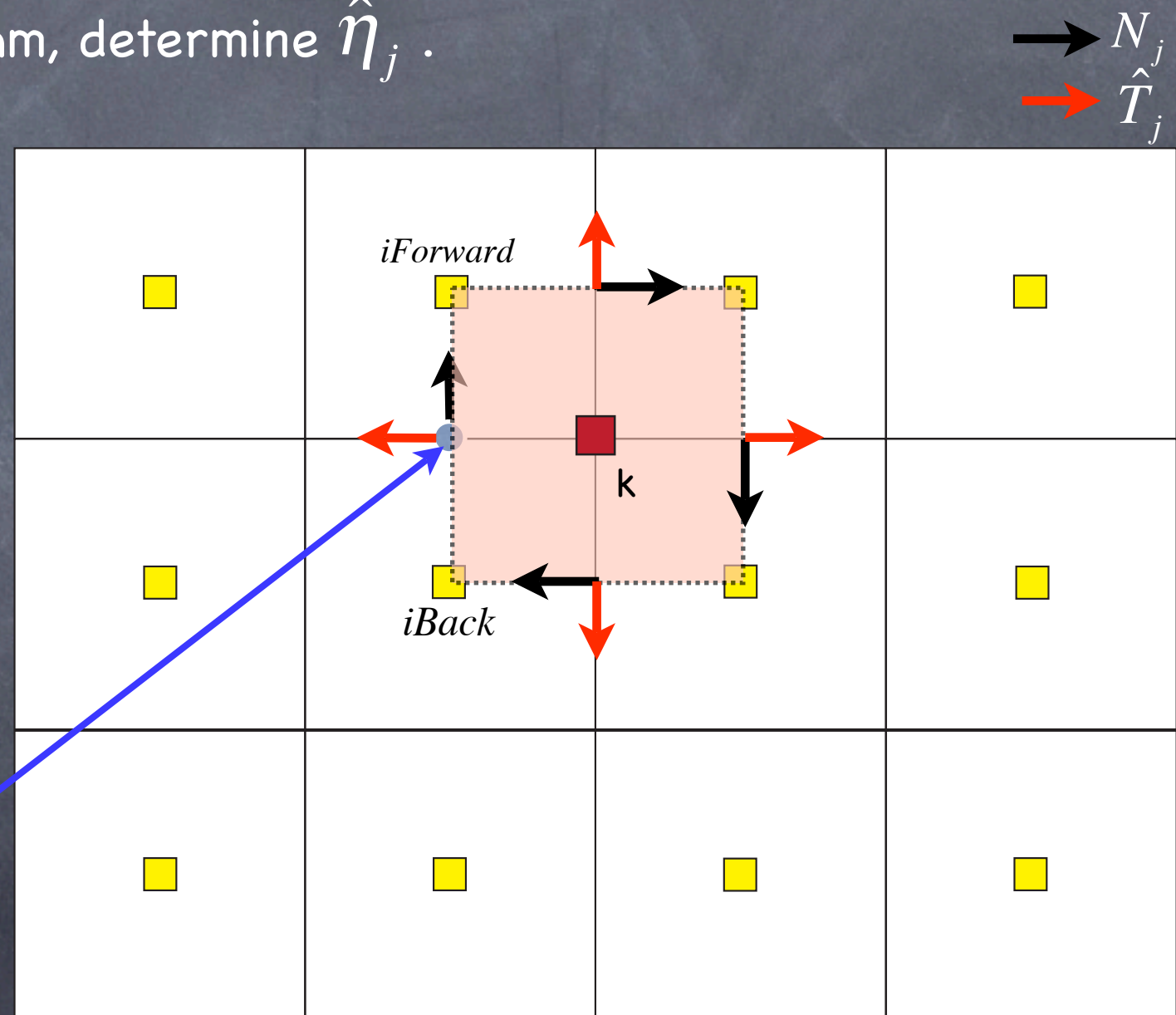


Transport-based approach for slaving velocity to an evolving vorticity field.

- 1) At $t=0$, given the velocity field determine absolute vorticity at k points.
- 2) Reconstruct T velocities (shown in red).
- 3) Using your favorite transport algorithm, determine $\hat{\eta}_j$.
- 4) Use this $\hat{\eta}_j$ in the momentum eq.

At the end of the time step ($n+1$), the curl of the velocity field at $n+1$ plus the Coriolis parameter is equal (i.e. within machine round-off error) to the absolute vorticity at $n+1$.

$\hat{\eta}_j$



Summary, 1 of 3

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On the one hand, high order reconstructions will inevitably lead to over/under shoots. The primary question to ask is: How will these over/under shoots impact the chemistry component, the cloud parameterization and so on. Is the simulation really “accurate” if the high-order transport algorithm damages the quality of the parameterizations?

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On the one hand, high order reconstructions will inevitably lead to over/under shoots. The primary question to ask is: How will these over/under shoots impact the chemistry component, the cloud parameterization and so on. Is the simulation really “accurate” if the high-order transport algorithm damages the quality of the parameterizations?

On the other hand, limiting (either via fluxes or reconstruction) will inevitably lead to something close to 1st-order accuracy when the limiting is active. The primary question to ask is: How important is enforcing monotonicity, positive definite or other bounds on the transport? Is a smooth simulation of tracer transport worth the reduction in formal accuracy?

Summary, 2 of 3

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Climate simulations with 10 to 100 tracer quantities are now common, and the number will only grow in time. There is no reason to think that the same algorithm to compute \hat{Q} is appropriate for all tracer fields. Different schemes, along with different limiting options, will likely lead to a better overall simulation per computational cost.

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If the above is considered, attention needs to be given to insure mass/tracer consistency for all tracers. Are all transport methods consistent with the single mass evolution equation?

Summary, 3 of 3

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Monotone (or otherwise) limited transport schemes add diffusion that is variable in time and space. A “good” transport scheme will add that diffusion only when and where it is required. By construction, flux-limited transport schemes enhance the down-gradient flux.

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Monotone (or otherwise) limited transport schemes add diffusion that is variable in time and space. A “good” transport scheme will add that diffusion only when and where it is required. By construction, flux-limited transport schemes enhance the down-gradient flux.

Many (most?) discrete models of tracer transport include ad hoc horizontal mixing, such as Laplacian or biharmonic smoothing that are generally active at all time at all places. The use of flux-limited transport can reduce the need for ad hoc smoothing.